Visualisation of Cost Landscapes

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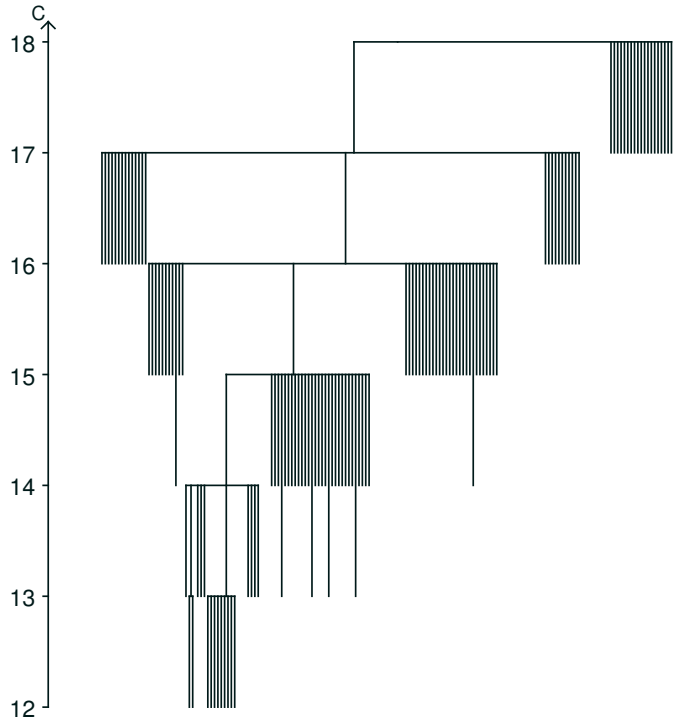
Work in collaboration with Jonathan Hallam and Will Benfold

Outline

1. Optimisation Problems
2. Cost Landscapes
3. Barrier Trees
4. Example Instances
5. Mapping Configurations
6. Modelling the Problem



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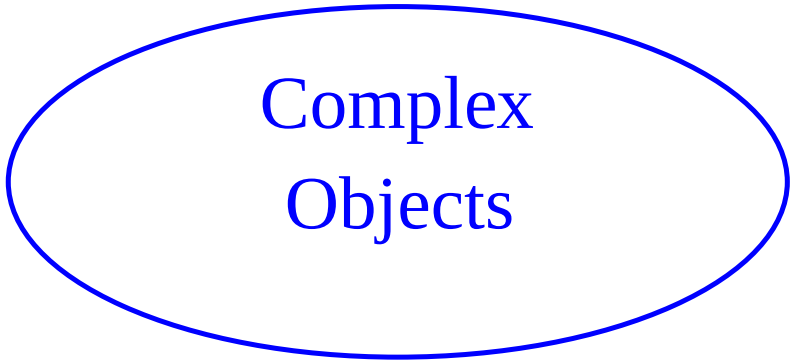

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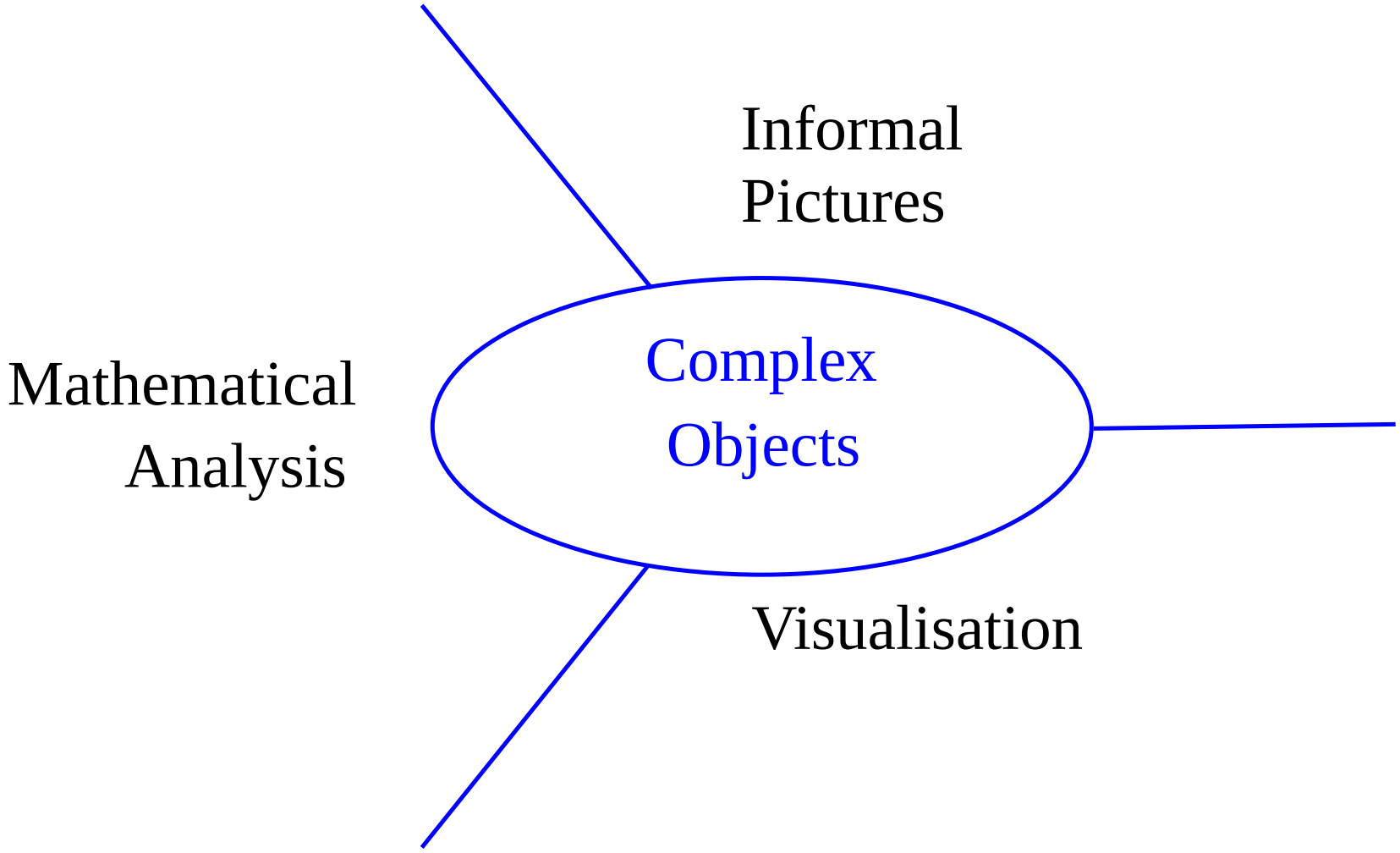

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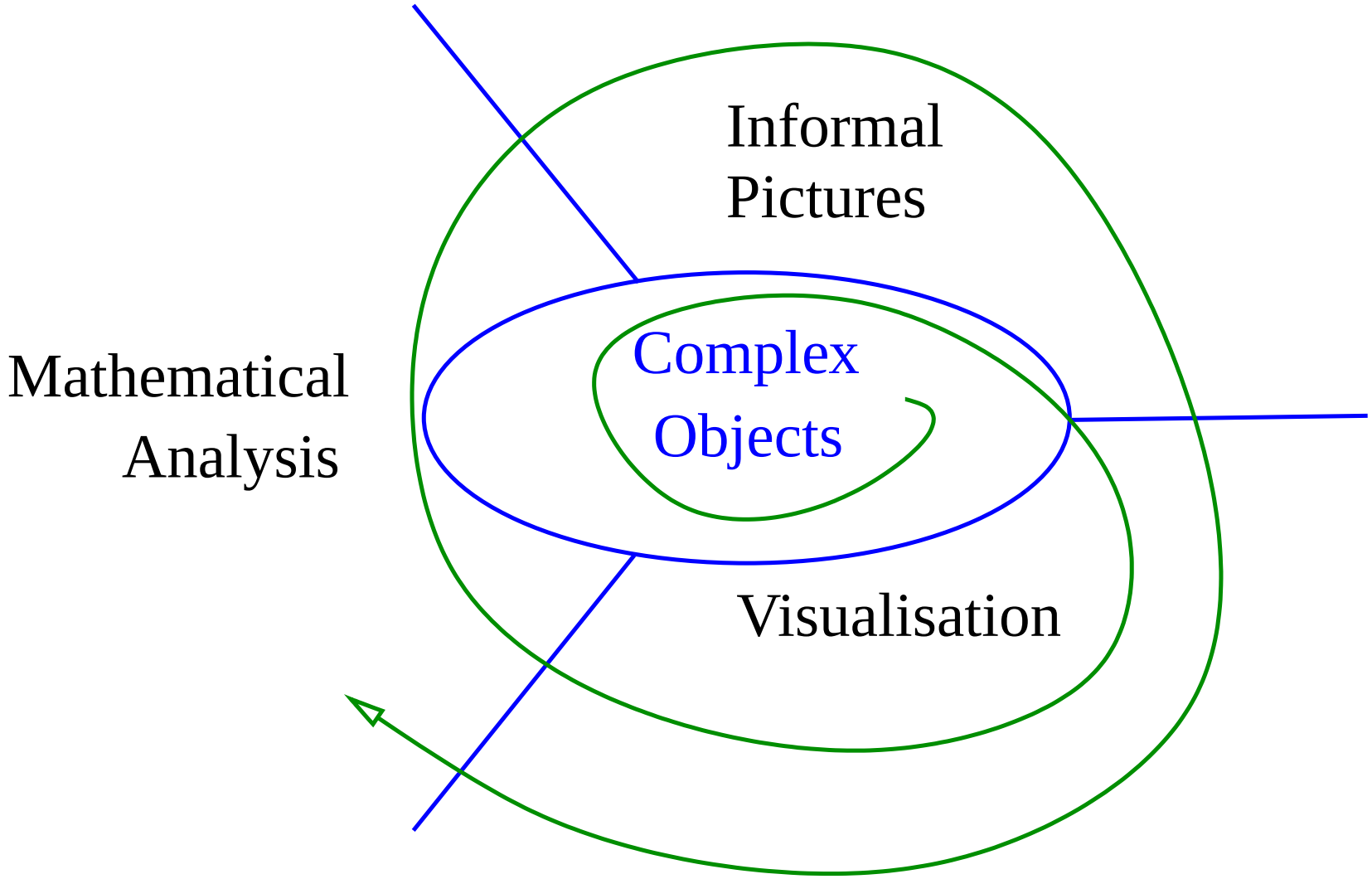

Combinatorial Optimisation Problems

- Set view: $\mathcal{S}$—'the search space'

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- Consider mainly degenerate problems $|f(\mathcal{S})| \ll |\mathcal{S}|$

Example: Max-Sat

- Given n Boolean variables $X_i \in \{T, F\}$
- M disjunctive clauses, e.g.

$$c_1 = x_1 \vee \neg x_2 \vee x_3$$
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Max-Sat Problems

- Arises naturally in digital circuits
- Many planning problems reduce to Max-Sat
- Any non-deterministic Turing machine can be reduced to a SAT problem—Cook's theorem
- Factorisation can be solved using a SAT solver

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Machine Learning Example

- Perceptron is a classic learning machine for performing binary classification

- Given a data set $\mathcal{D} = \{\boldsymbol{x}_i, c_i\}_{i=1}^{P}$

  - $\boldsymbol{x}_i$—n-dimensional input pattern
  - $c_i \in \{-1, 1\}$—class label

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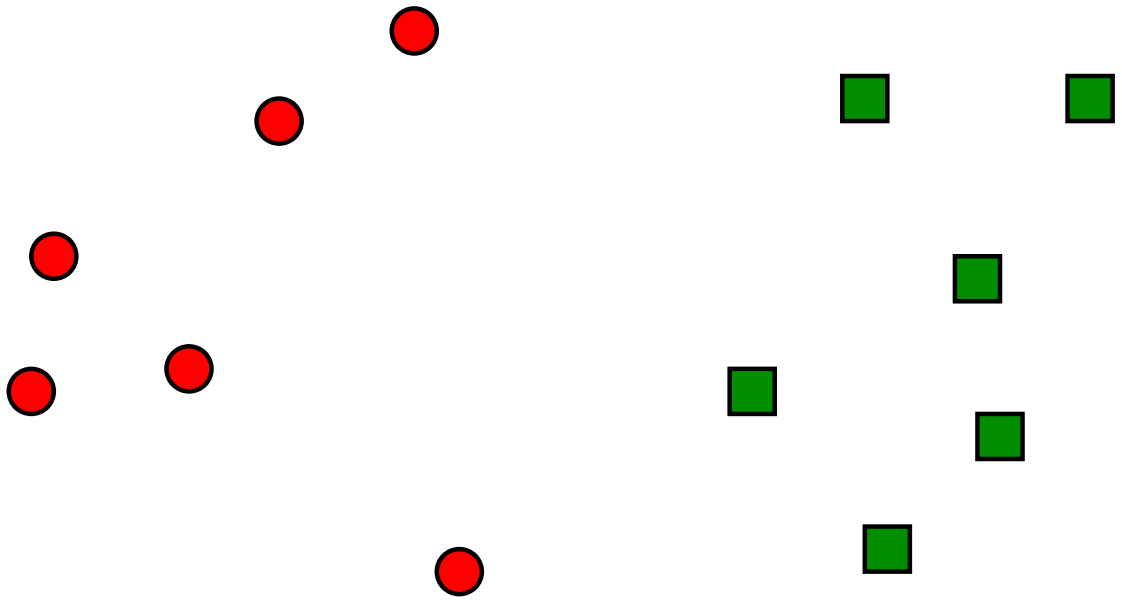

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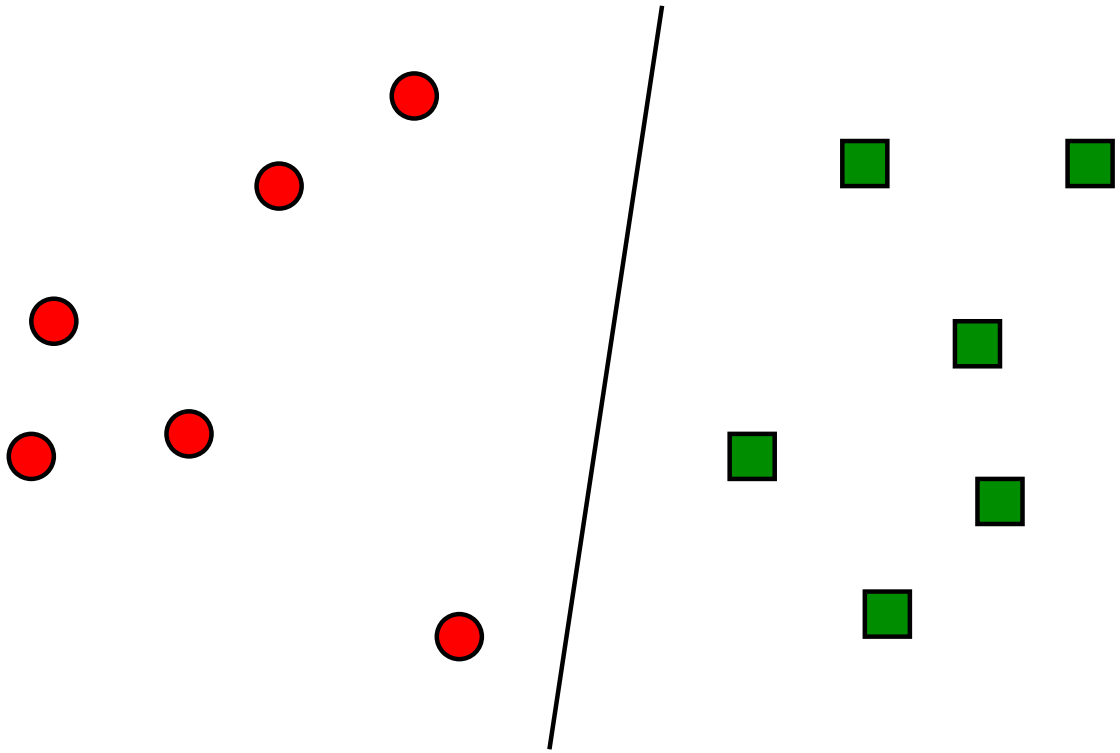

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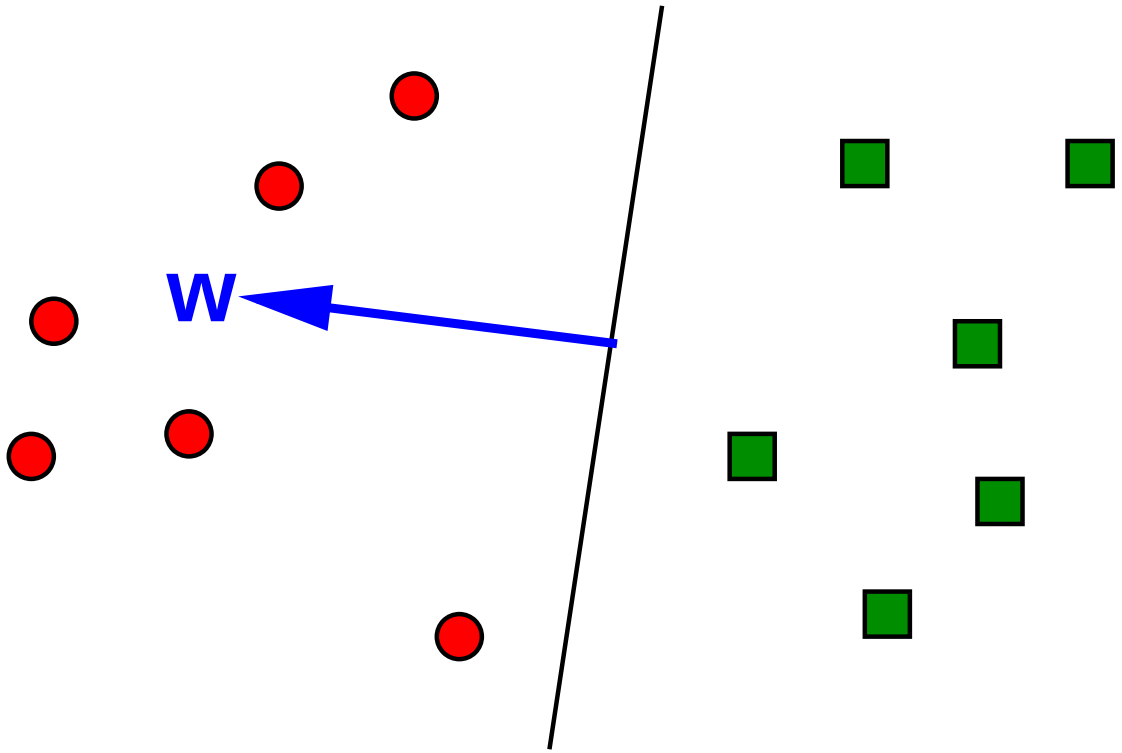

Ising Perceptron

- Weight vector is strongly constrained $\boldsymbol{w} = \{-1, 1\}^n$
- Problem becomes NP-Hard (integer programming problem)
- Both Max-Sat and the Ising perceptron have a lot of structure not captured by the set view of optimisation problems

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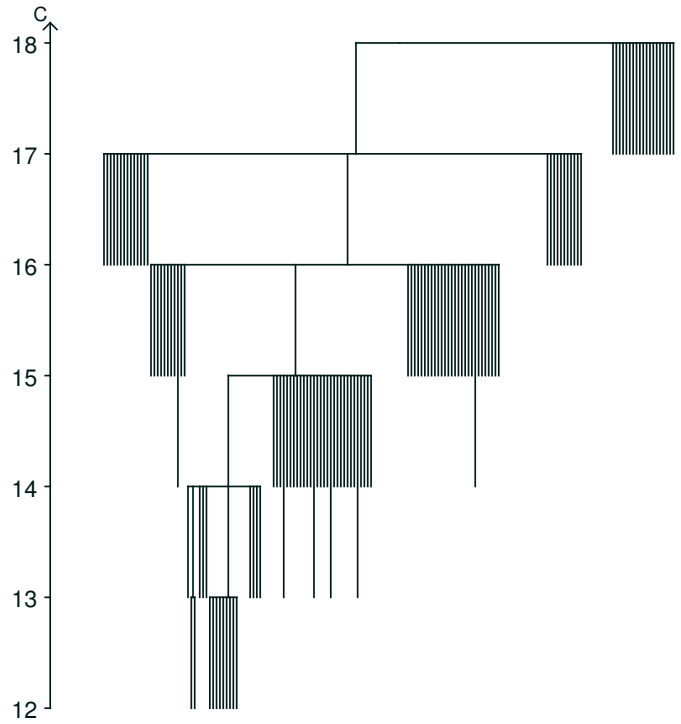

Neighbourhood

- We can introduce a topology to a search space by defining a neighbourhood function $\mathcal{N} : \mathcal{S} \mapsto 2^{\mathcal{S}}$

- Neighbourhoods are often connected with local search operators

  $\mathcal{N}(\boldsymbol{x})$ is the set of configurations we can move to from $\boldsymbol{x}$

- Key Heuristic: Neighbouring configurations are more likely to have a similar cost than random configurations

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Hamming Neighbourhood

- A natural neighbourhood for binary strings is the Hamming neighbourhood
- Configurations differing at a single site are neighbours

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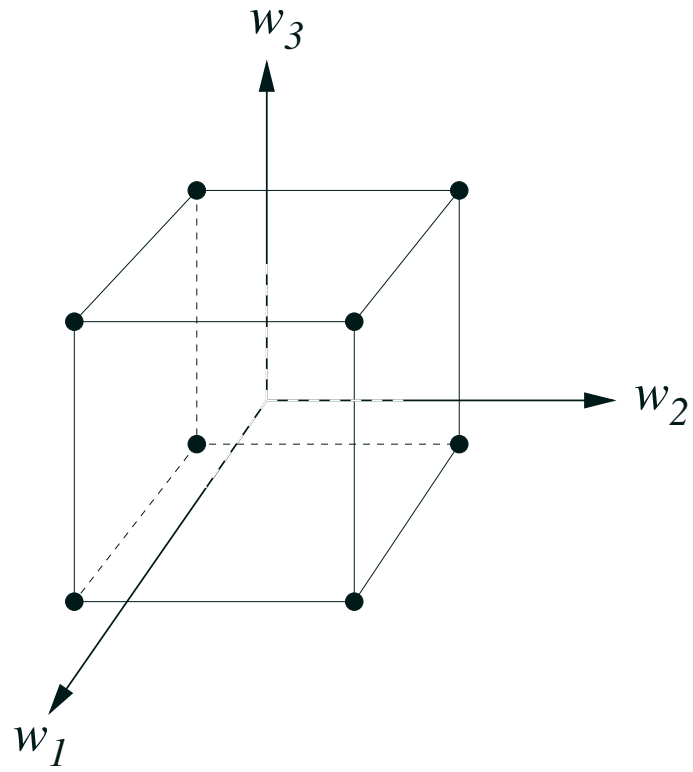
Hypercube Topology

- The Hamming neighbourhood induces a hypercube topology on the search space of binary strings



3D Binary String Search Space

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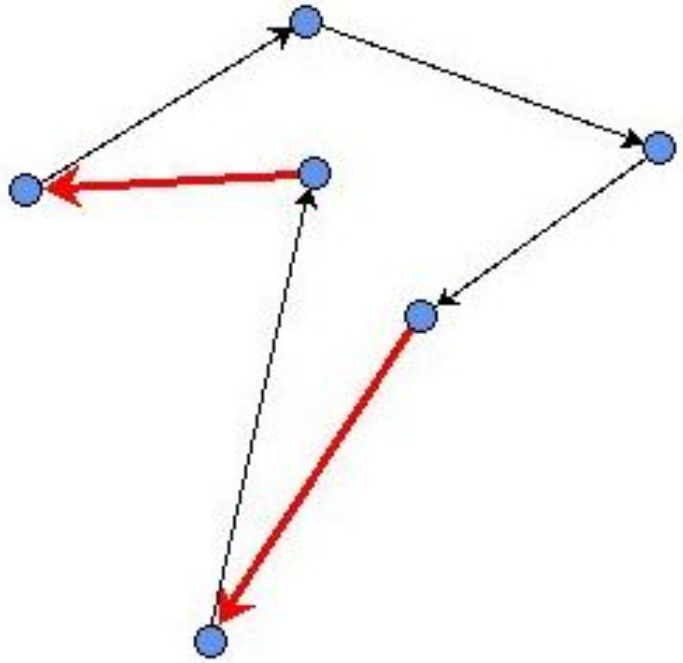

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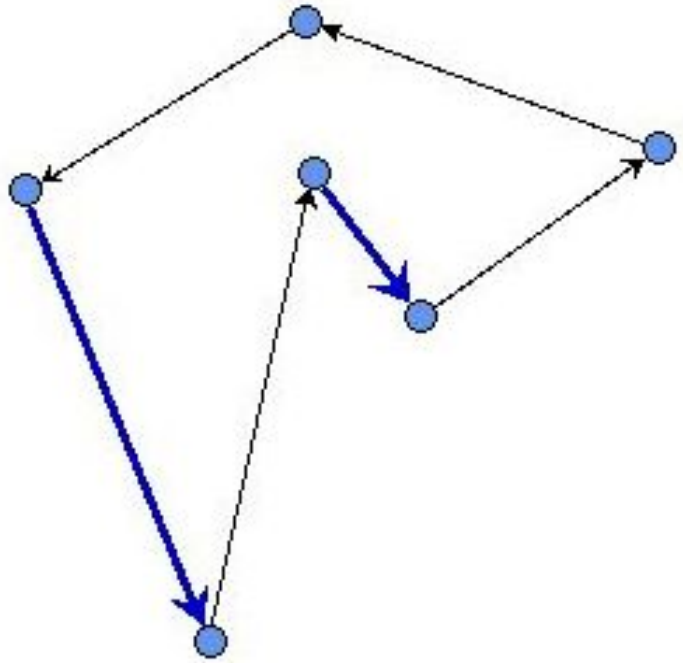

2-Opt neighbours

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- Cost function + Neighbourhood = Landscape

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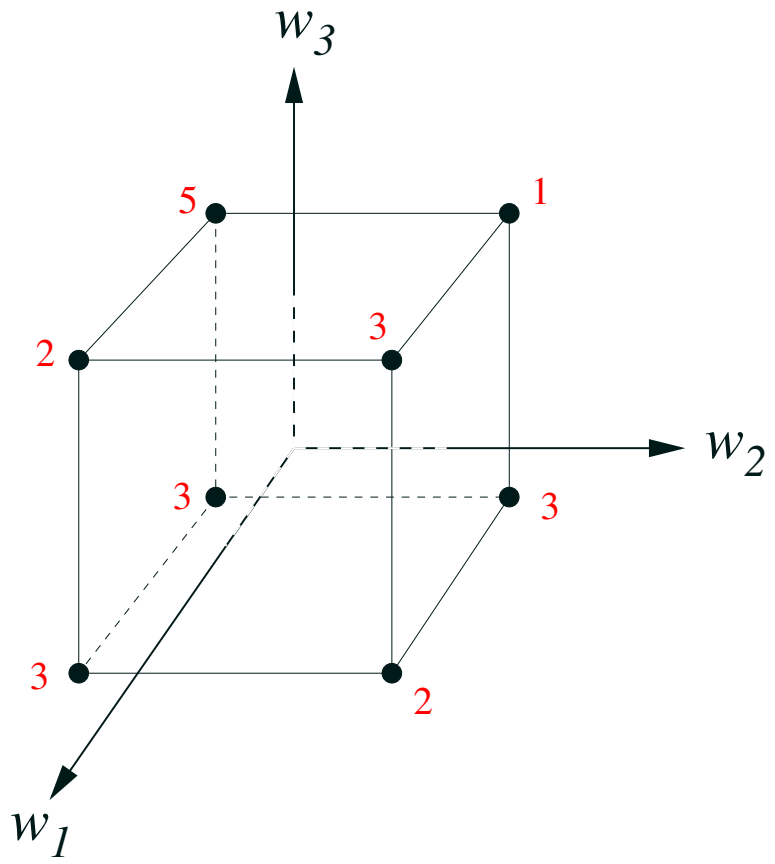

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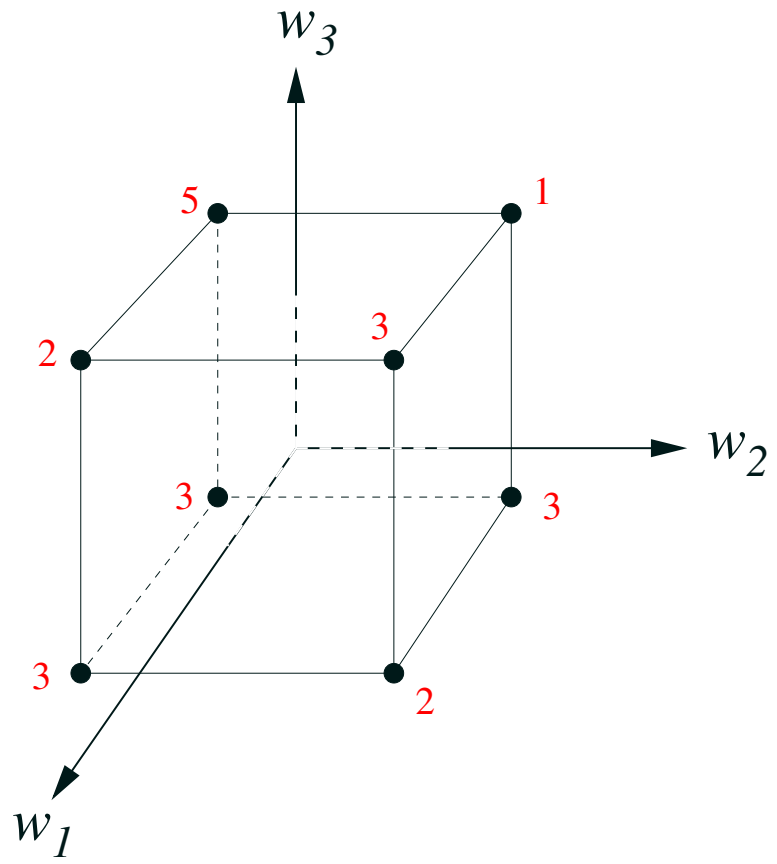

- Unfortunately difficult to visualise in high dimensions

Costs in the Ising Perceptron

Each input divides the search space in two

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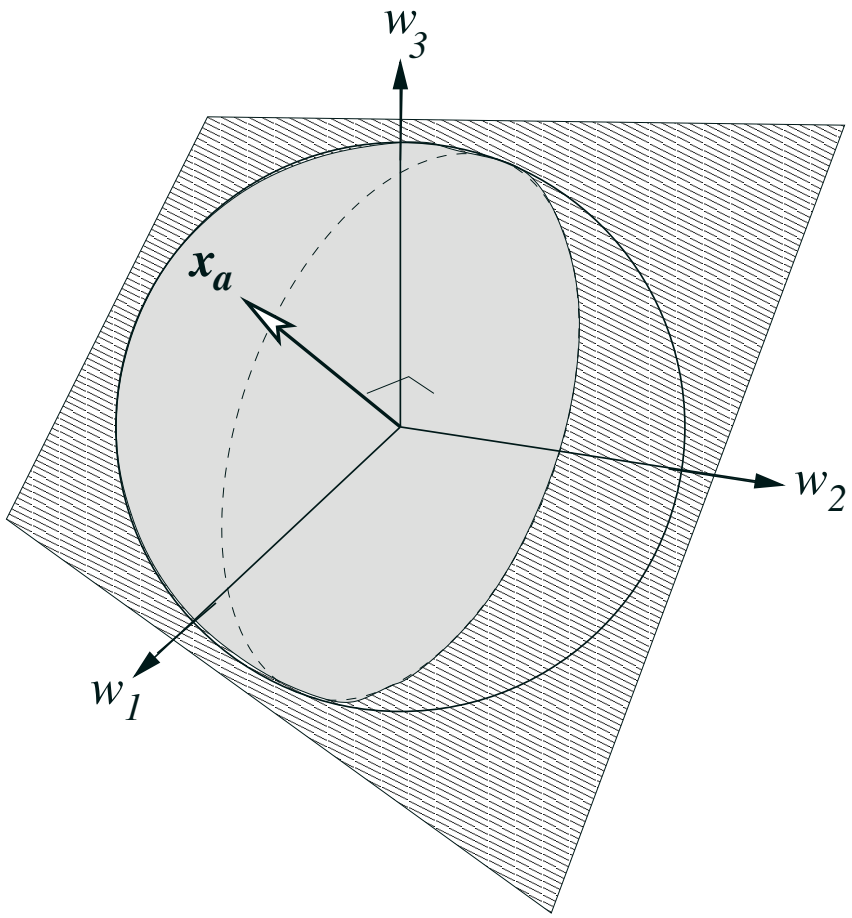

Correctly Classified Region

The set of inputs defines a cone on the hypersphere which correctly classifies all inputs

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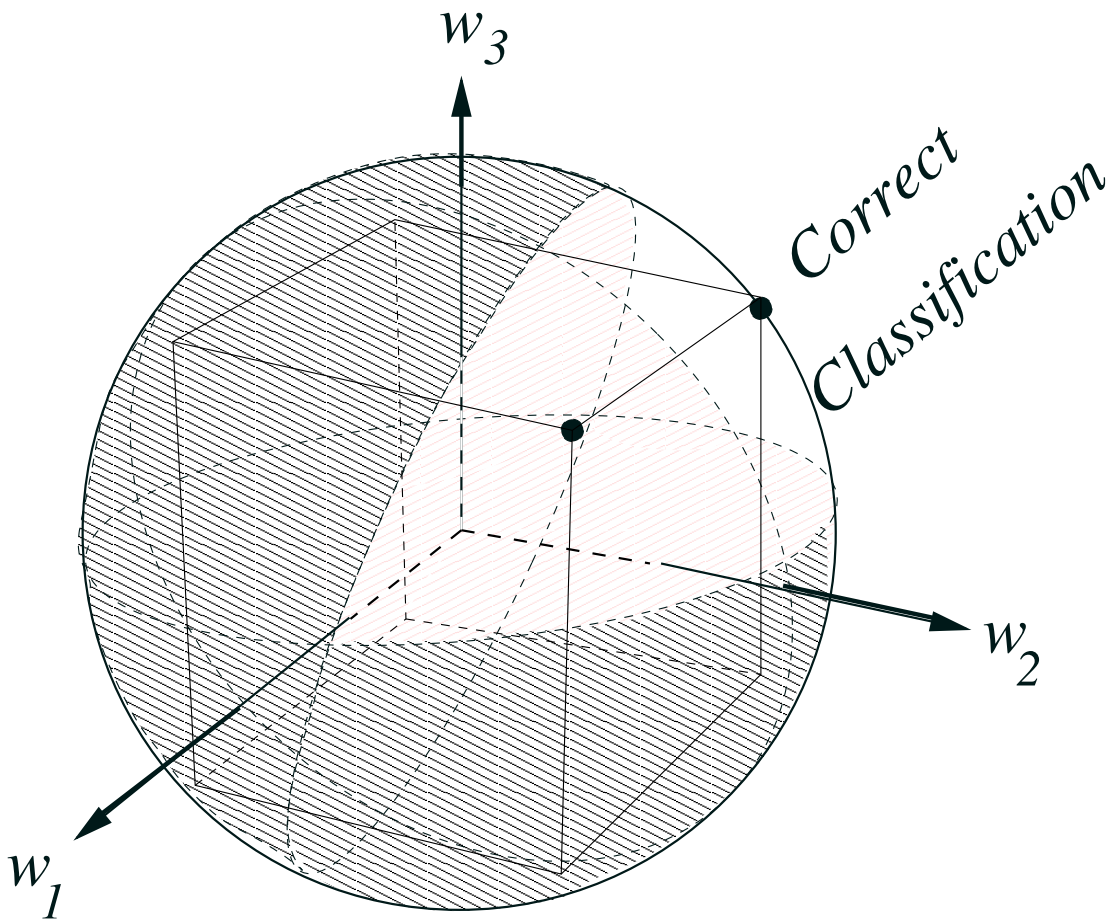

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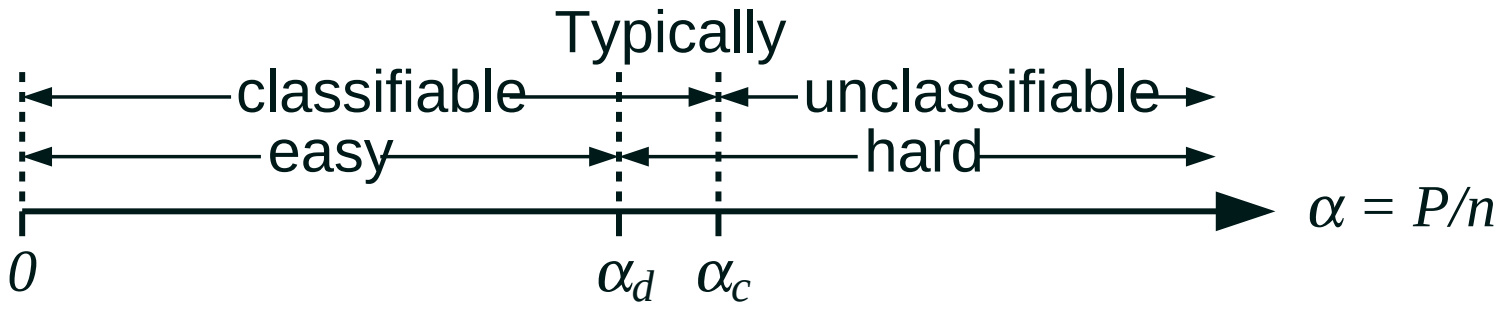

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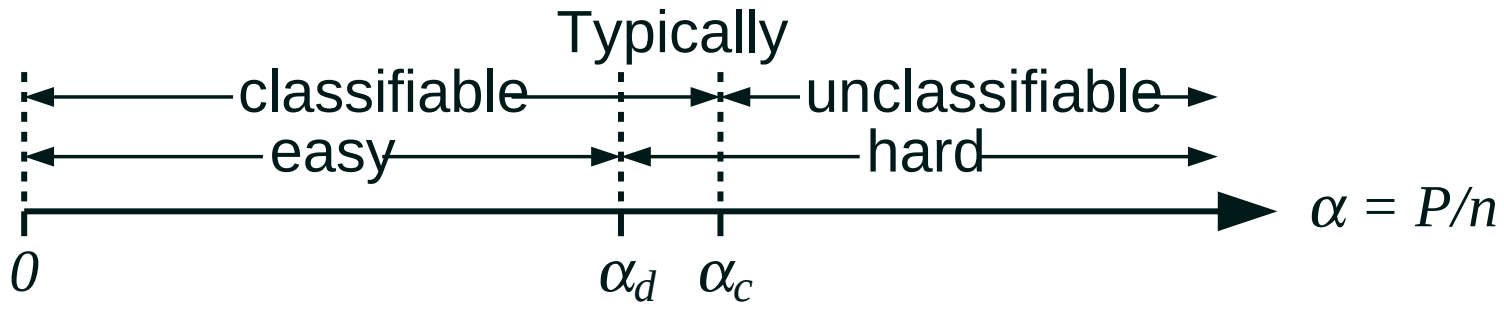
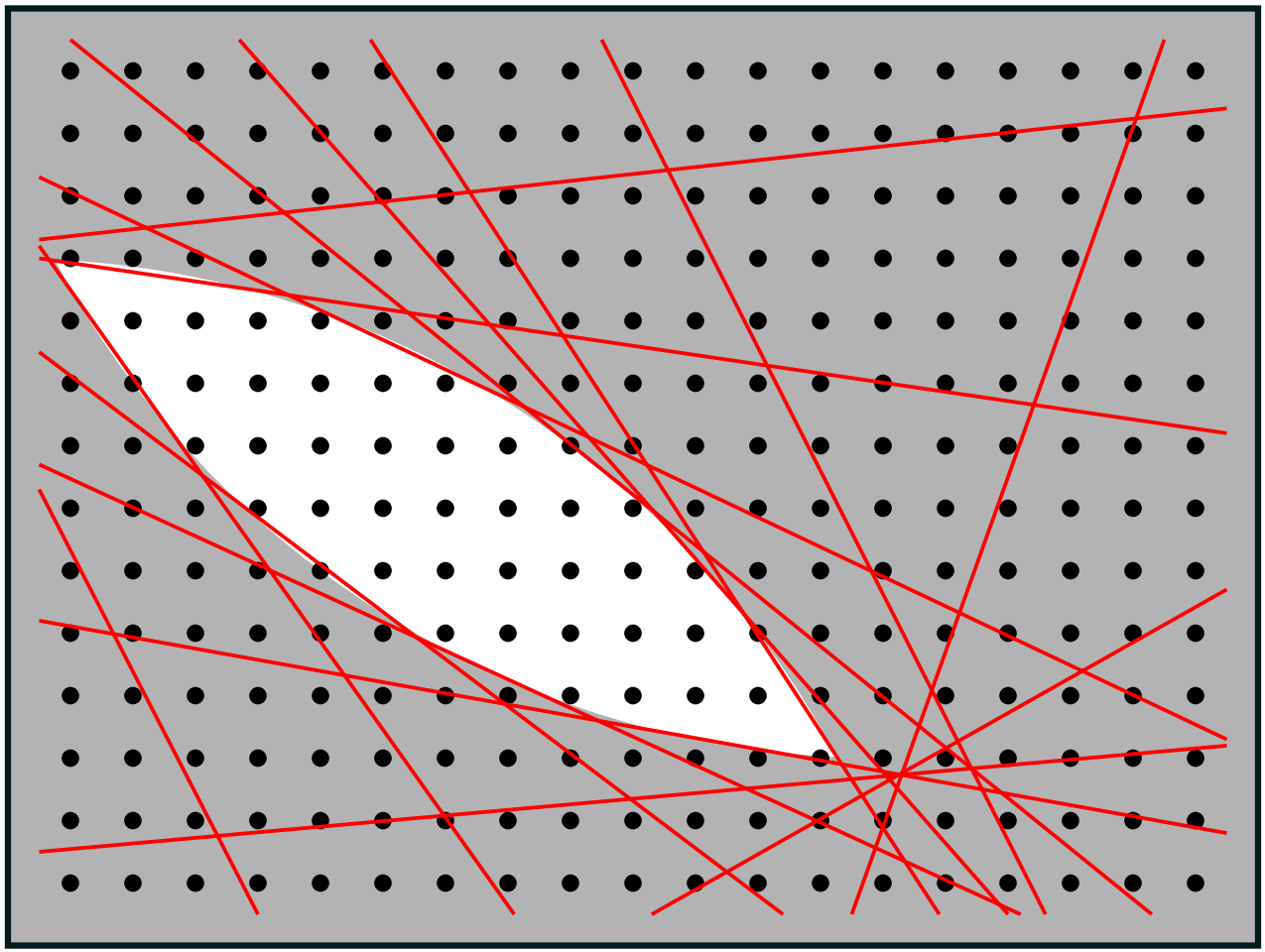


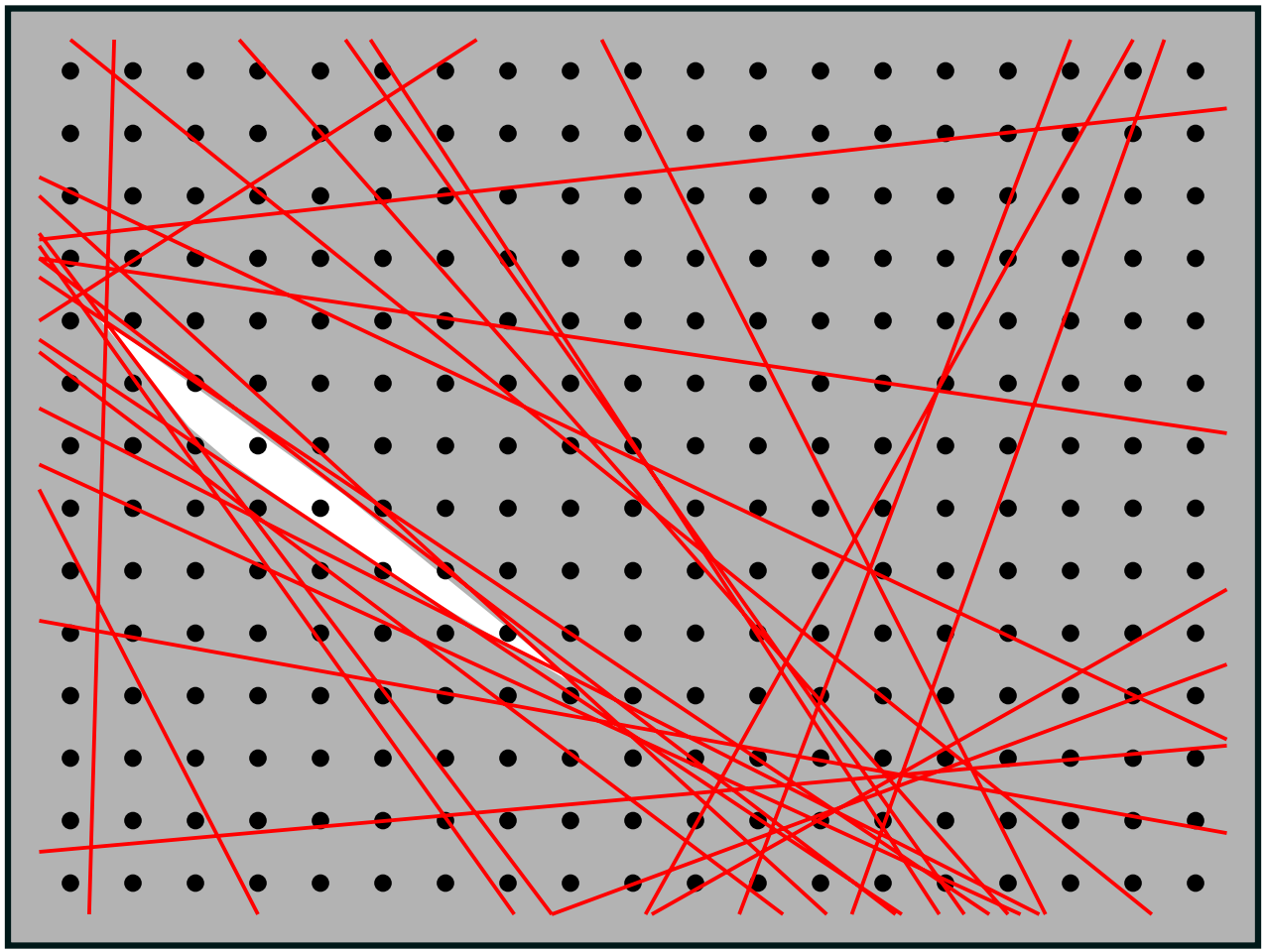
- Typically means that the exceptions become exponentially rare with n

Schematic representation of low α



Note that the real search space is high dimensional

Schematic representation at higher α



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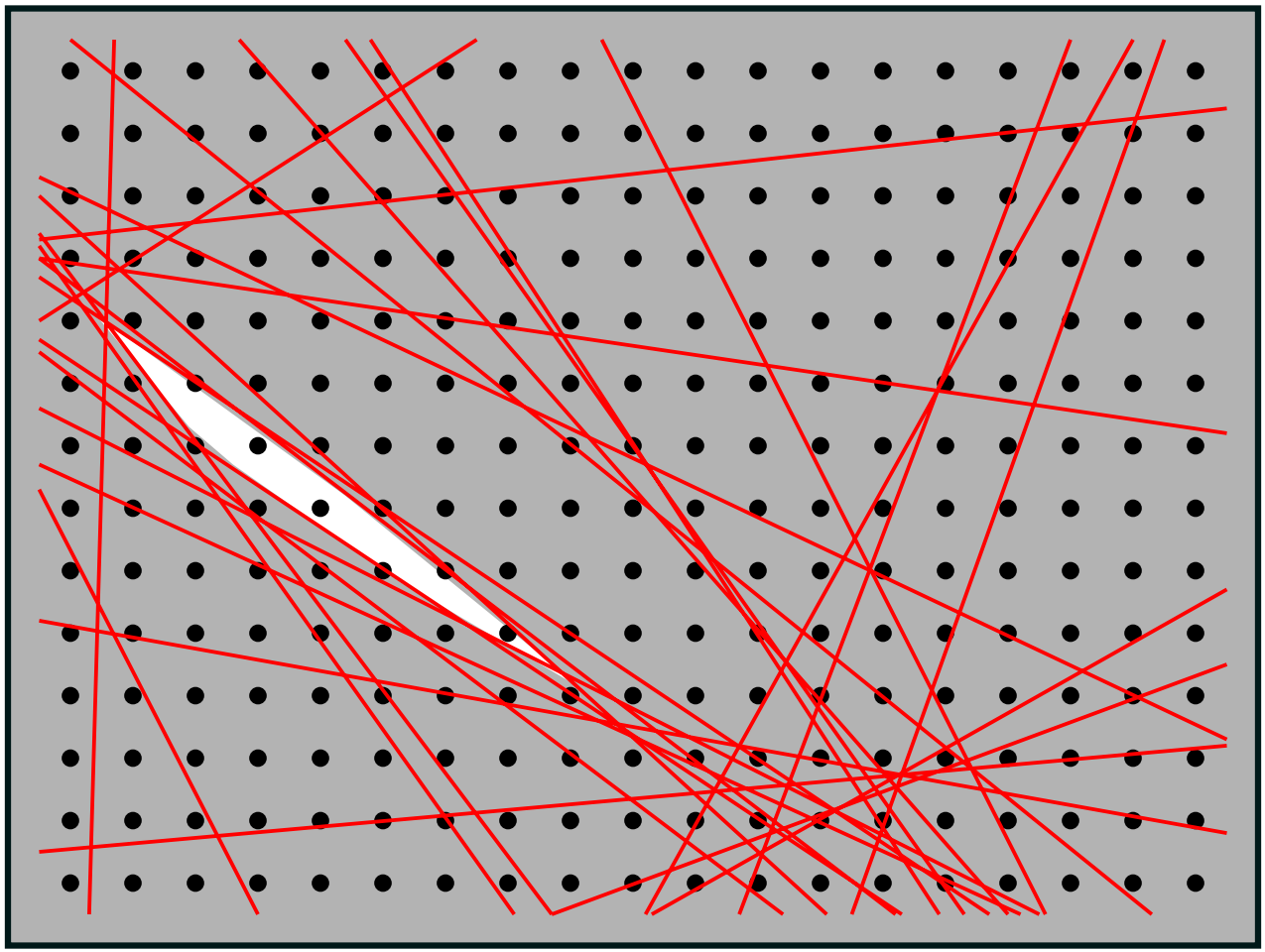

Solutions are typically disconnected

Replica Symmetry Breaking

- The problem becomes hard just as the solutions become disconnected
- The solutions can be a long way apart
- The solution space "shatters" into many local optima rather like a piece of glass
  - ⋆ shattering is random
  - ⋆ there are (exponentially) many local optima
  - ⋆ the sizes of the local optima differ dramatically
- In calculations this shattering causes "replica-symmetry breaking"

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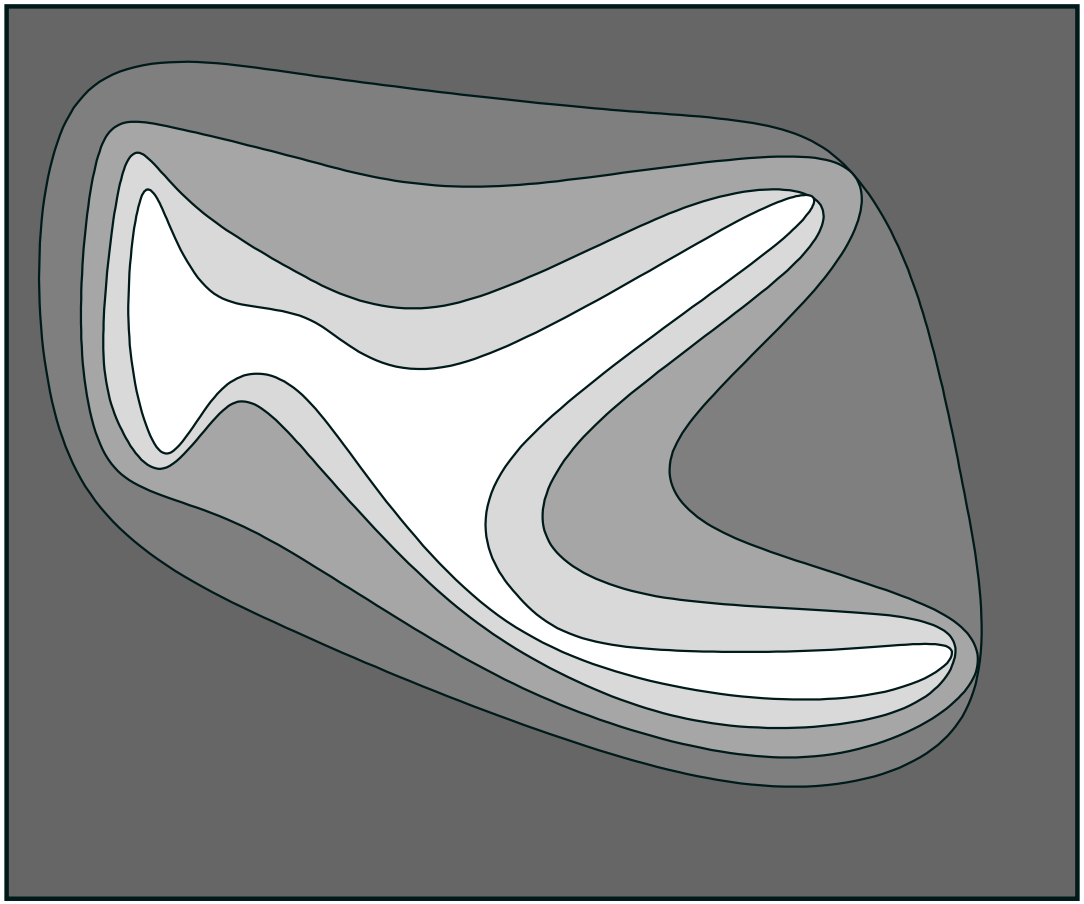
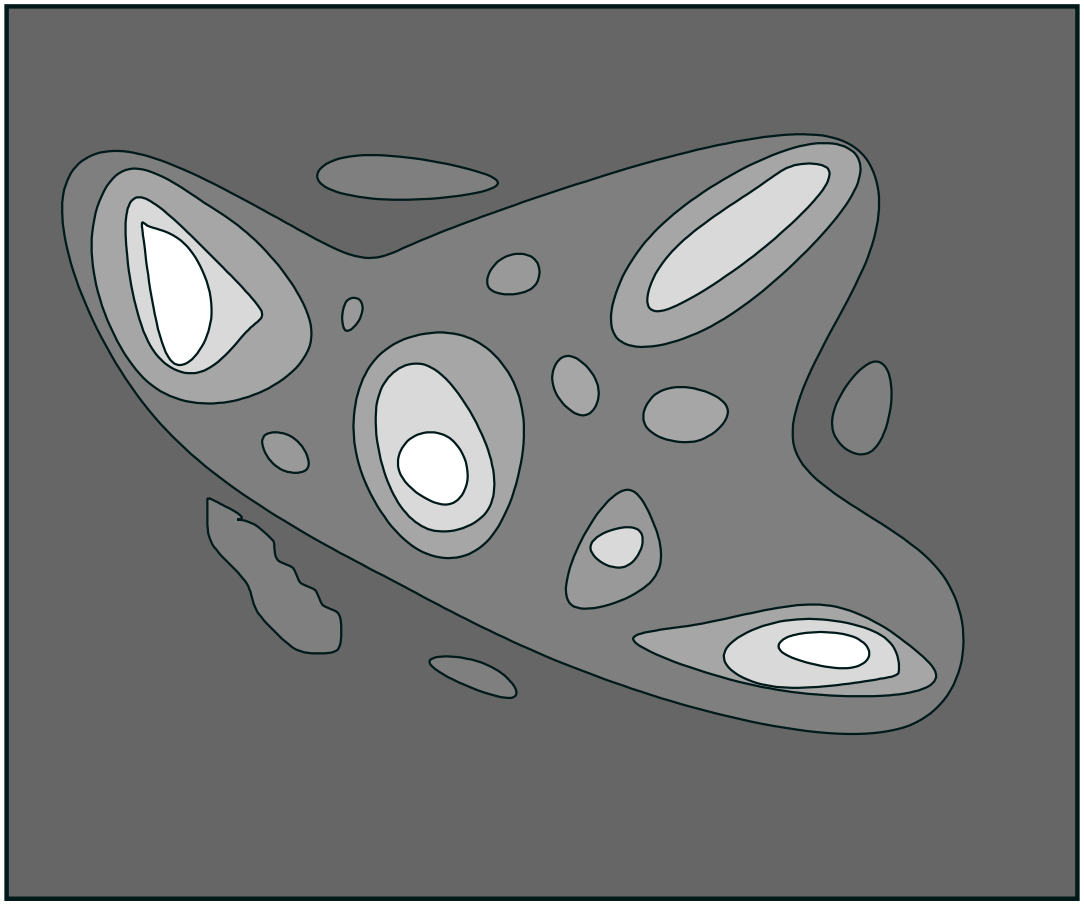


'Gradient' leads to global optima

Hard Phase

$\alpha > \alpha_d$



Ambiguous 'gradients'

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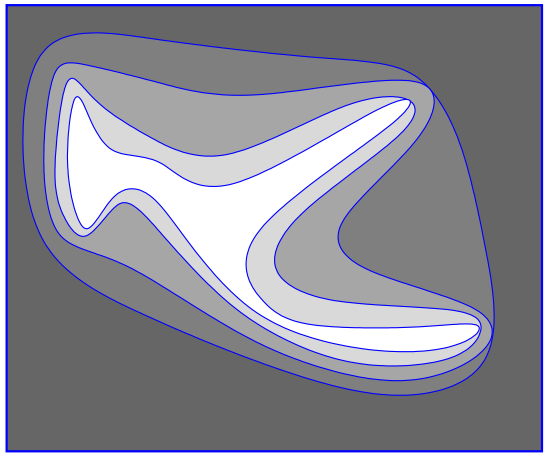

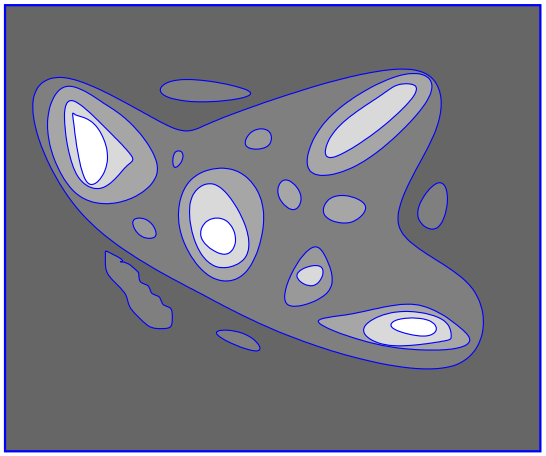

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- Usually there are exponential number of local optima
- Phase transition can be more complicated (e.g. number partitioning problem)

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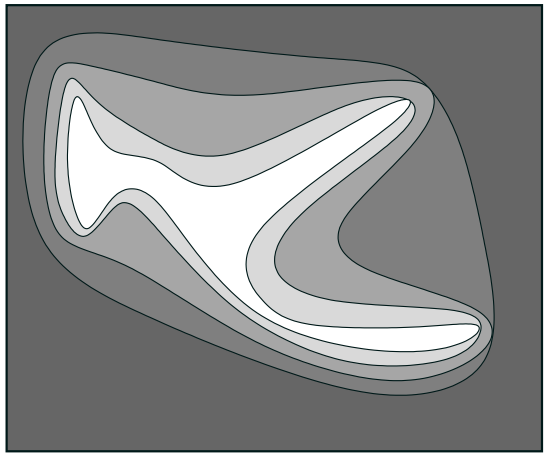

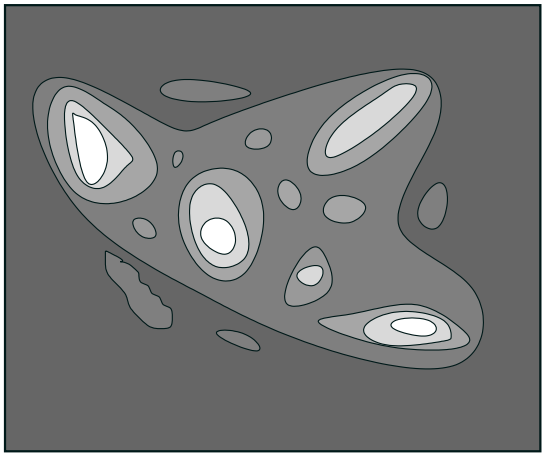

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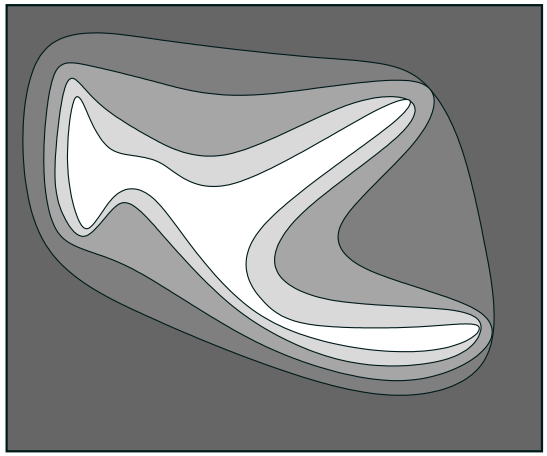

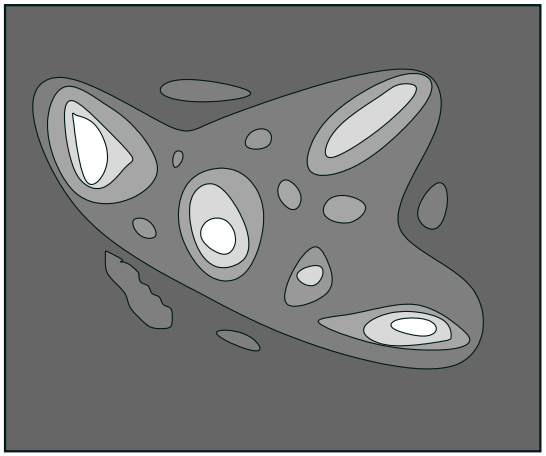

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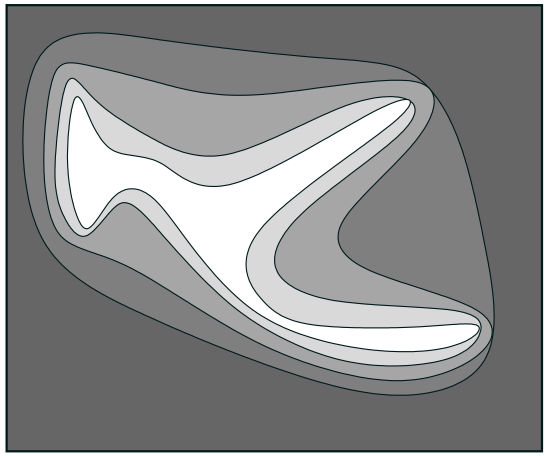
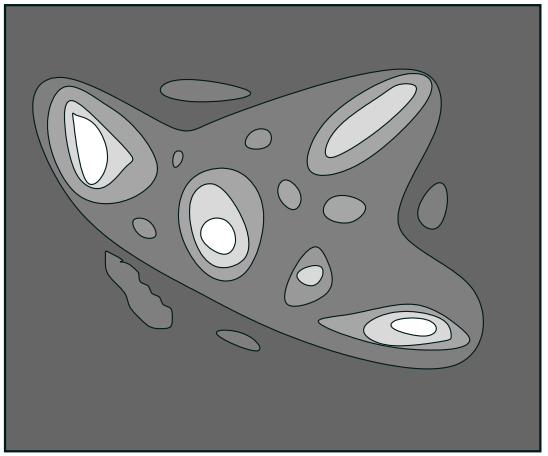
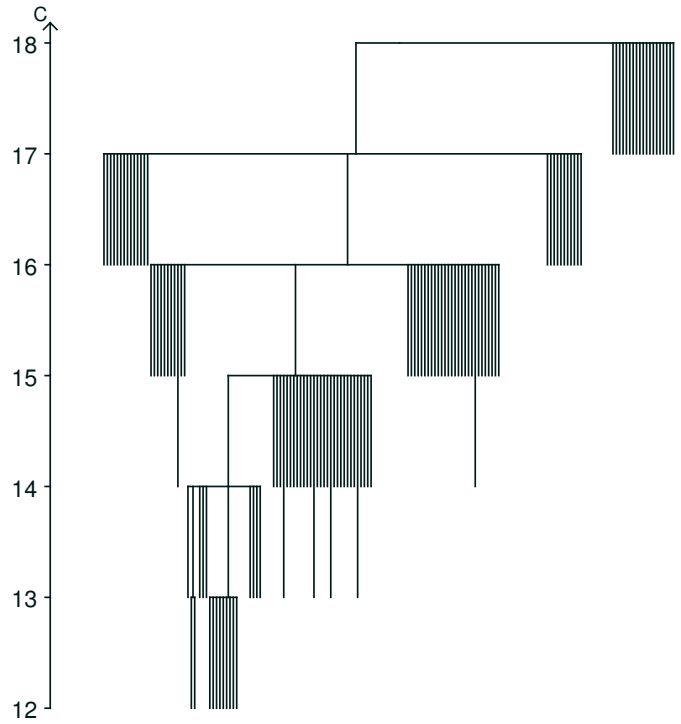




- Interested in high dimensional discrete problems
- Usually there are exponential number of local optima
- Phase transition can be more complicated (e.g. number partitioning problem)

Outline

1. Optimisation Problems
2. Cost Landscapes
3. Barrier Trees
4. Example Instances
5. Mapping Configurations
6. Modelling the Problem



Barrier Trees

- To help visualise the search space we can build a 'Barrier Tree'
- Leaves of the tree are local minima
- Merging vertices correspond to lowest cost saddle-points
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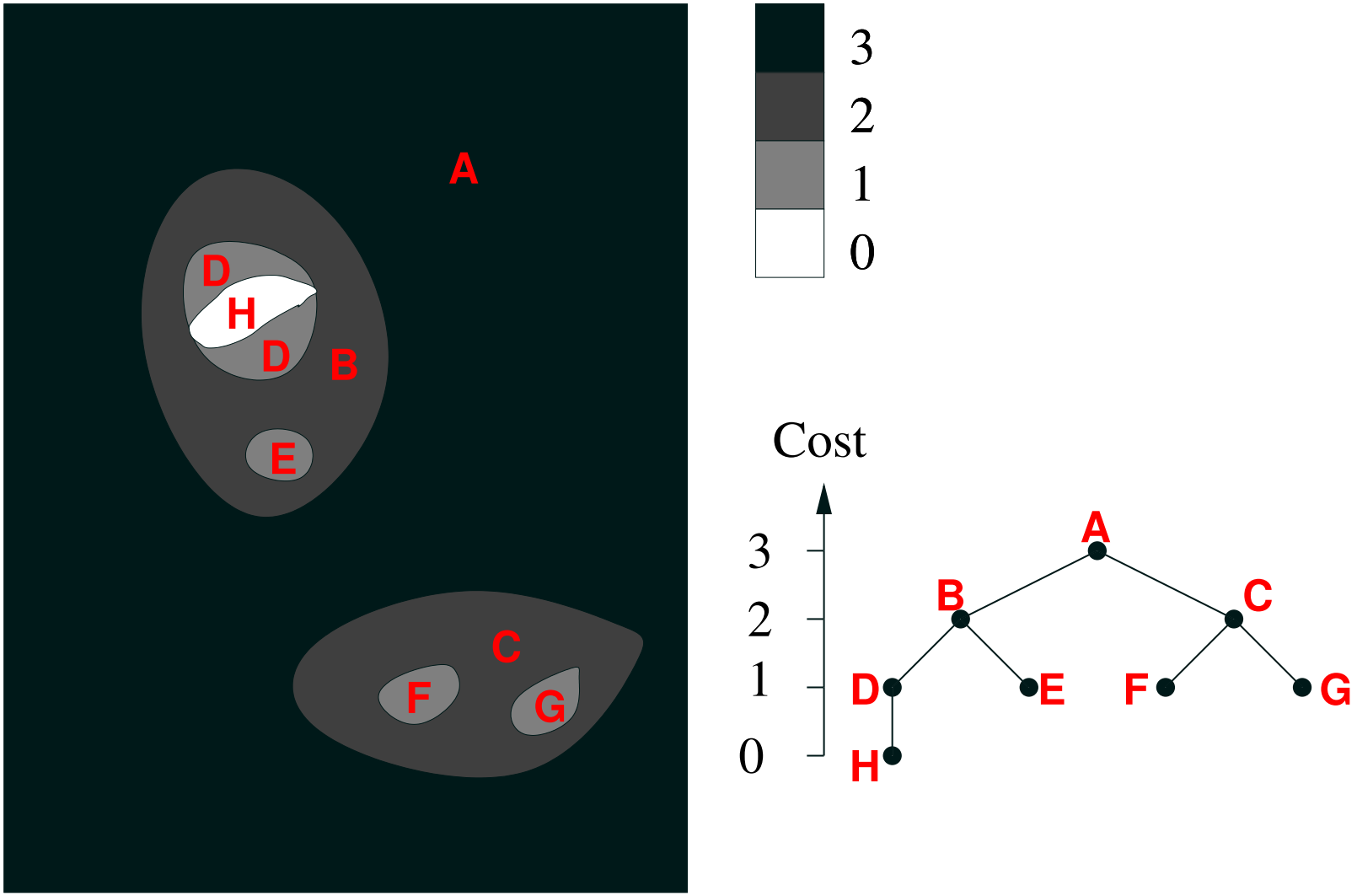
Example



Discrete Search Spaces

- To formalise these notion we define a path
  - ⋆ $\pi(\boldsymbol{x}, \boldsymbol{y}) = \left(\boldsymbol{x_i} \middle| \boldsymbol{x}_1 = \boldsymbol{x} \wedge \boldsymbol{x}_n = \boldsymbol{y} \wedge \boldsymbol{x}_{i+1} \in \mathcal{N}(\boldsymbol{x}_i)\right)$
  - ⋆ A sequence of Neighbouring configurations from $\boldsymbol{x}$ to $\boldsymbol{y}$
- Assume that the Neighbourhood relation is symmetric

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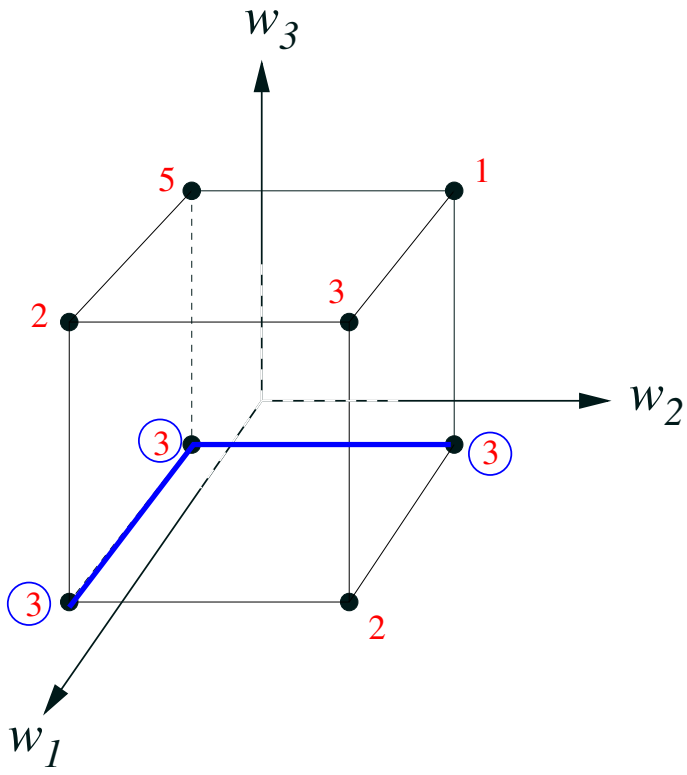
Level Connected Sets

- We define the level connectedness by the equivalence relation

$$\mathcal{LC} = \{(\boldsymbol{x}, \boldsymbol{y}) | \exists \pi(\boldsymbol{x}, \boldsymbol{y}) \wedge \forall \boldsymbol{x}_i \in \pi(\boldsymbol{x}, \boldsymbol{y}), f(\boldsymbol{x}_i) = f(\boldsymbol{x})\}$$



Limitation of Level Connectedness

- There are often a very large number of level-connected sets
- Consider the 'ones-max' problem where

$$f(\boldsymbol{x}) = \text{number of ones in } \boldsymbol{x}$$

- Every configuration is a level-connected set with a Hamming neighbourhood

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- In ones-max there are $N + 1$ level accessible sets

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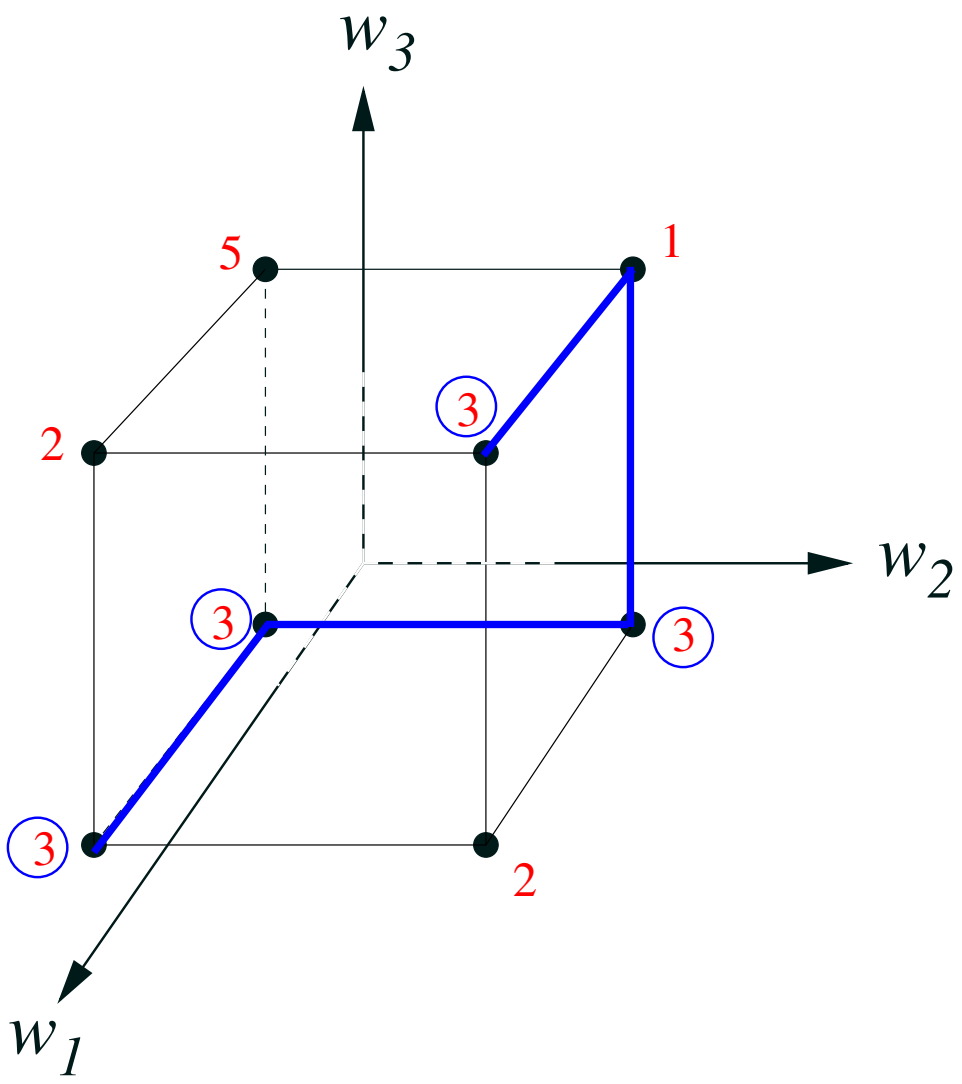

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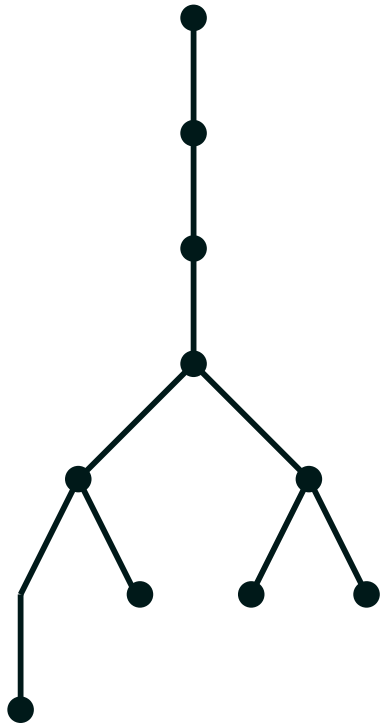

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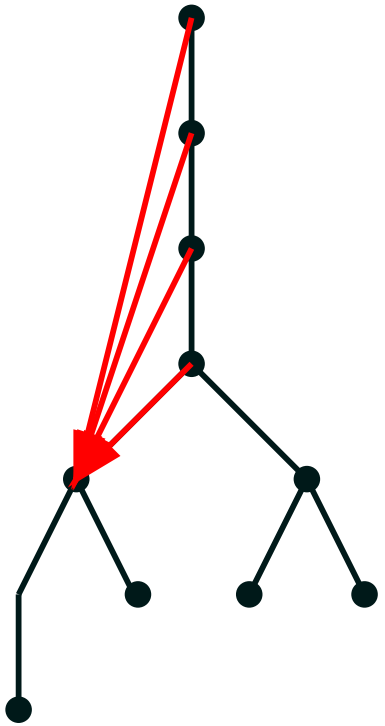

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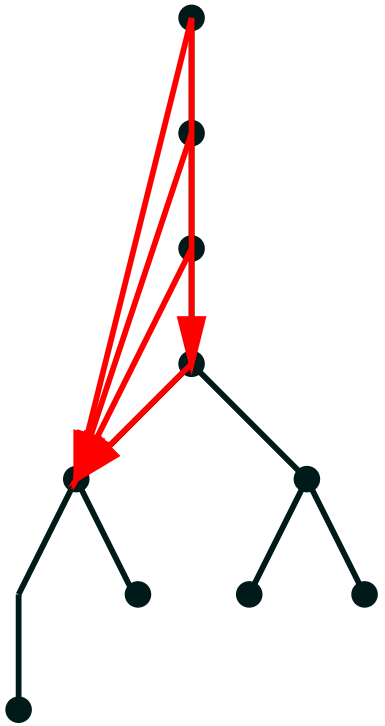

Computing Barrier Trees

- Finding the level-accessible sets and Barrier trees can be computed efficiently, $O(|\mathcal{S}| \times |\mathcal{N}|)$, using a flooding algorithm
- For larger problems we can compute the low-cost part of the Barrier tree using a modified branch and bound algorithm
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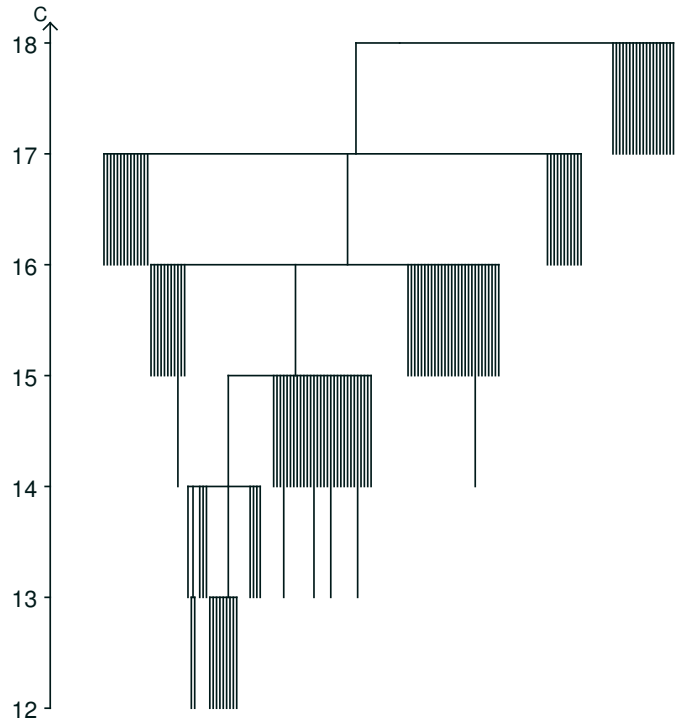
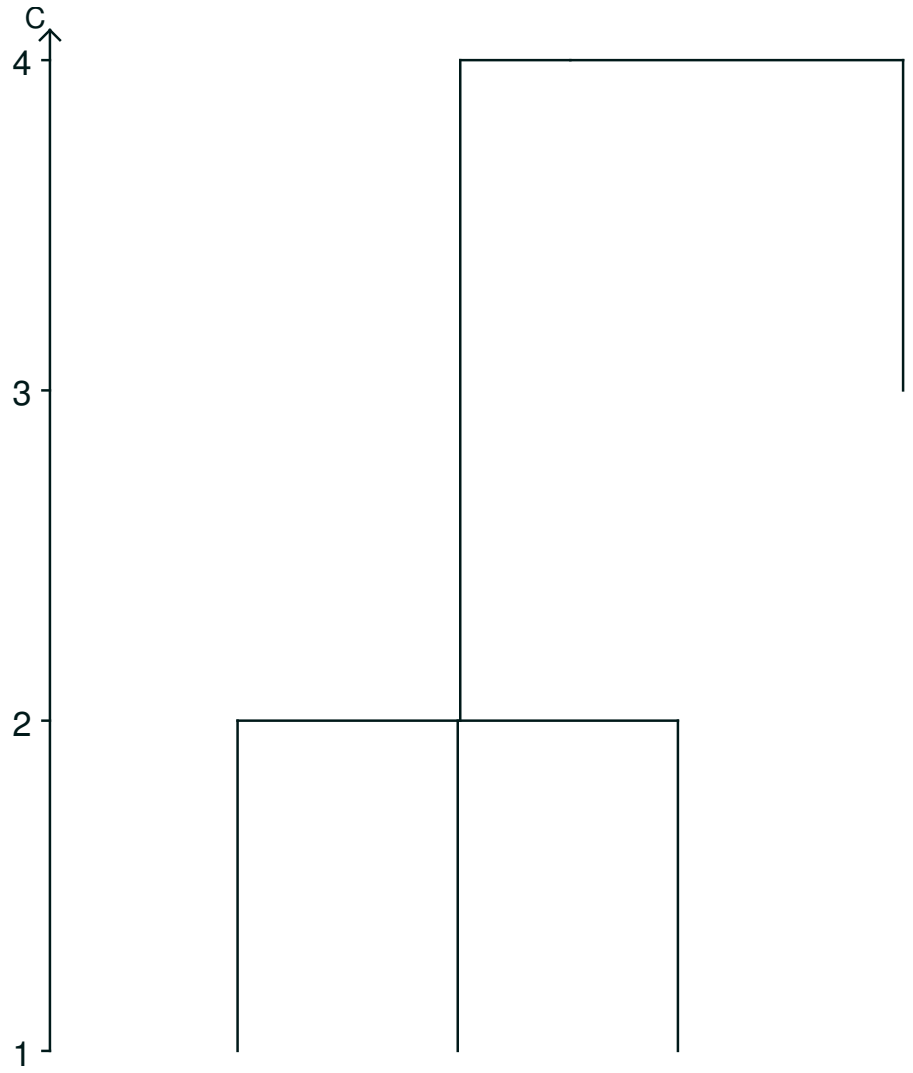
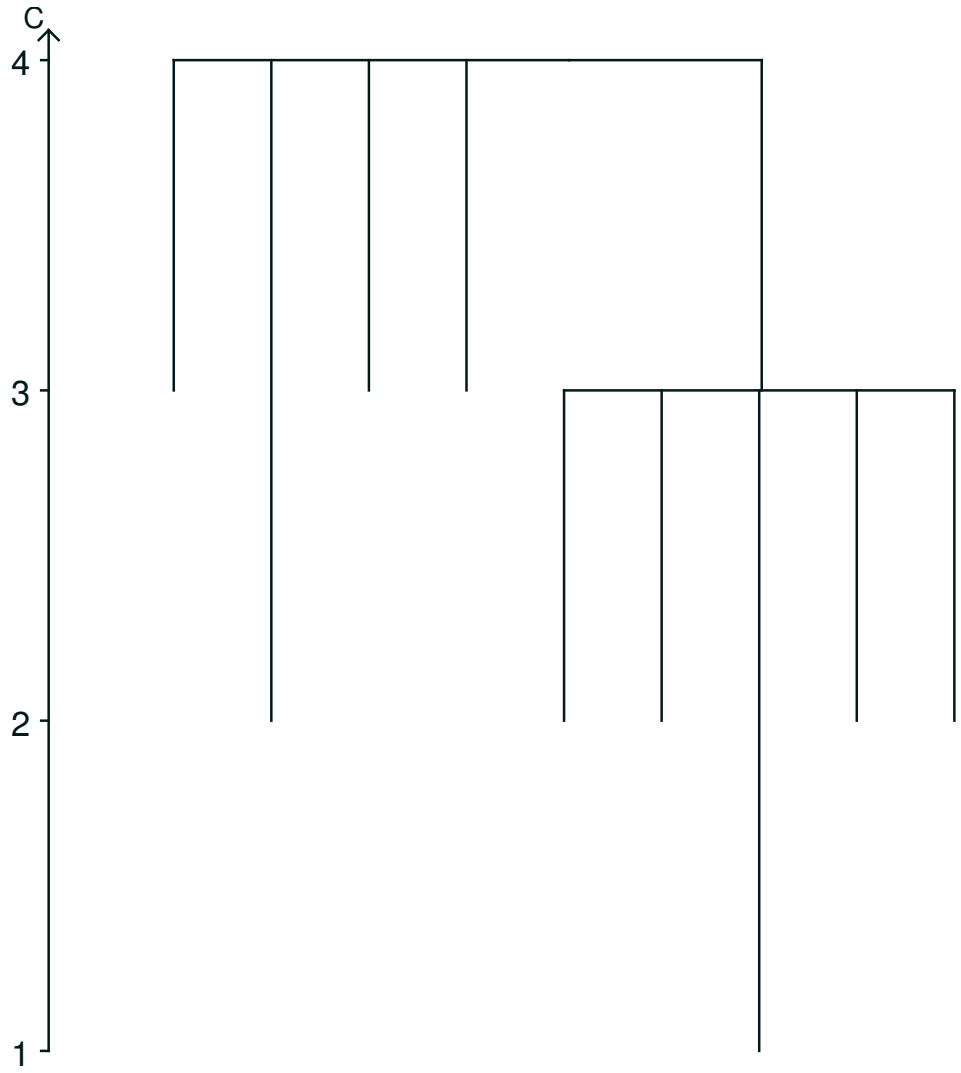


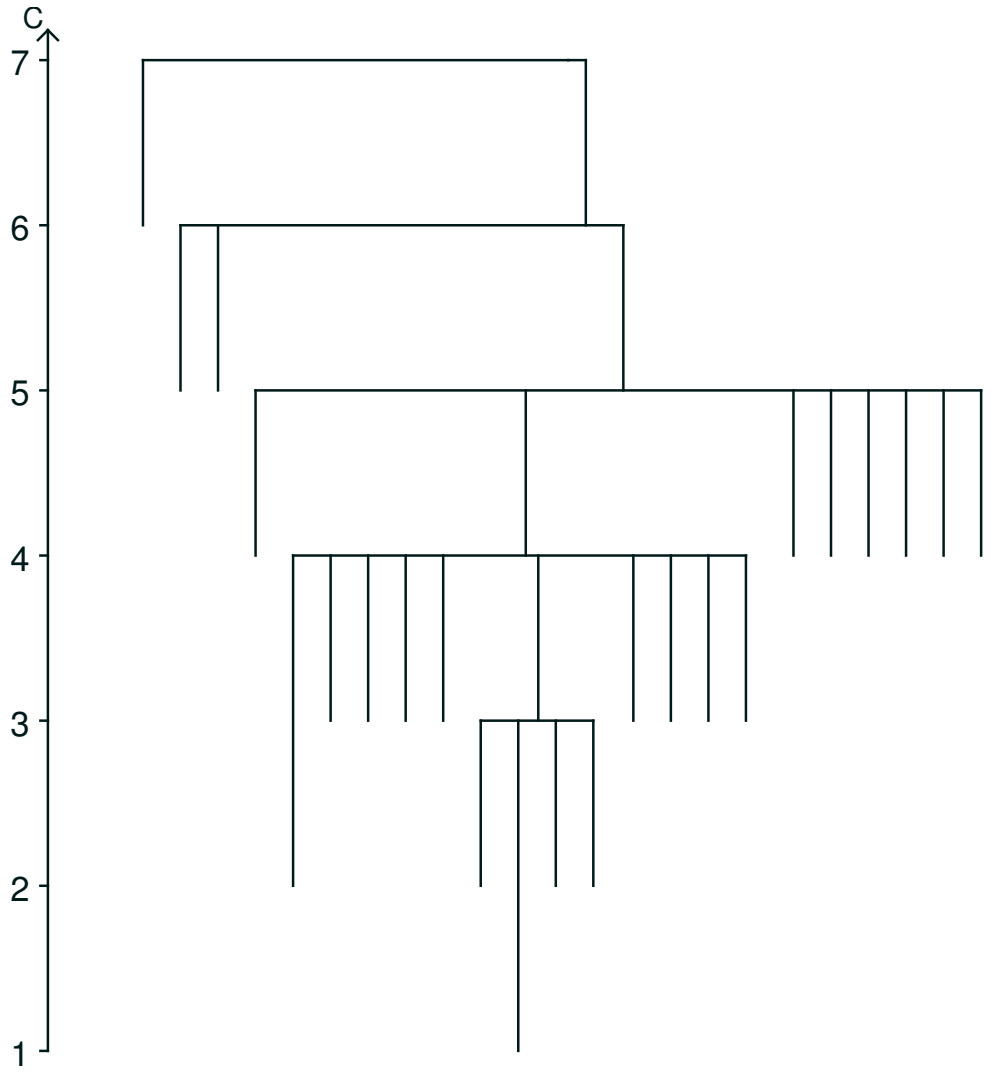
MAX-3-SAT $\alpha = M/N = 5$ $N = 10$



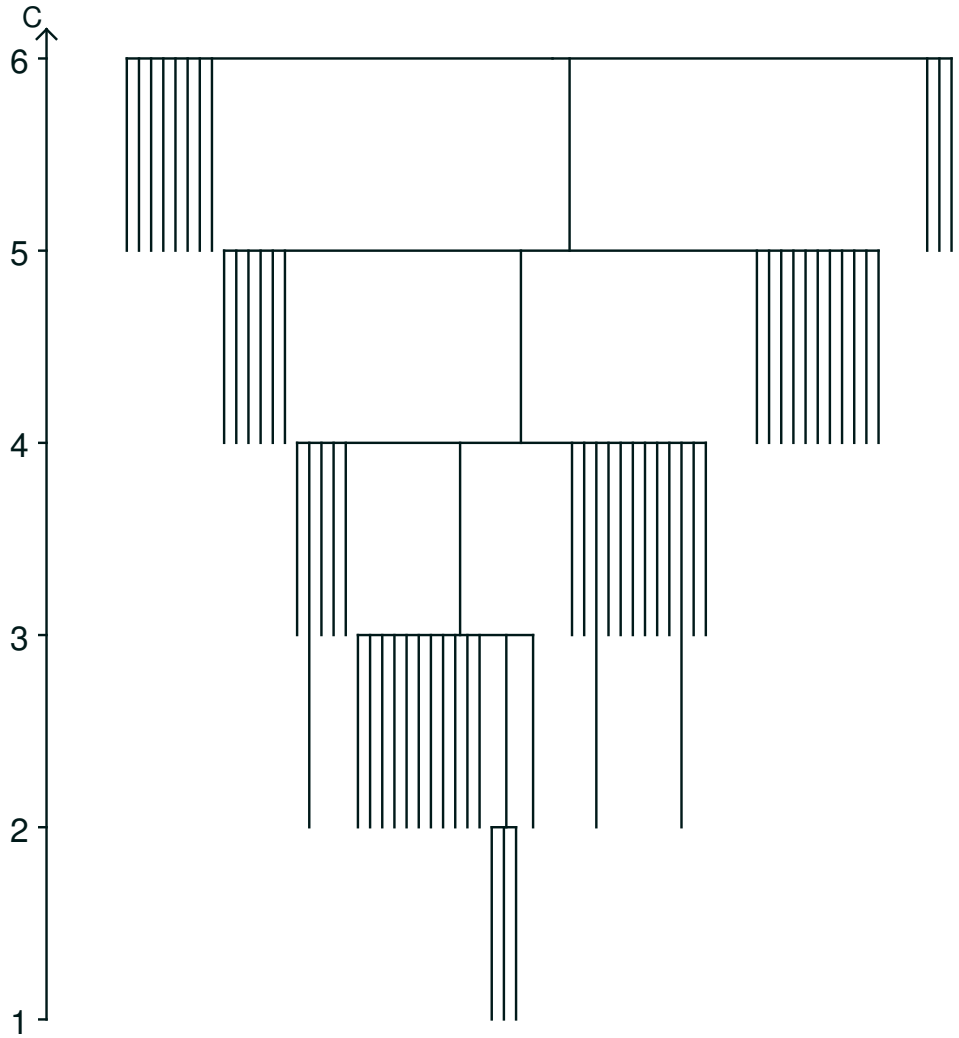
MAX-3-SAT $\alpha = M/N = 5$ $N = 20$



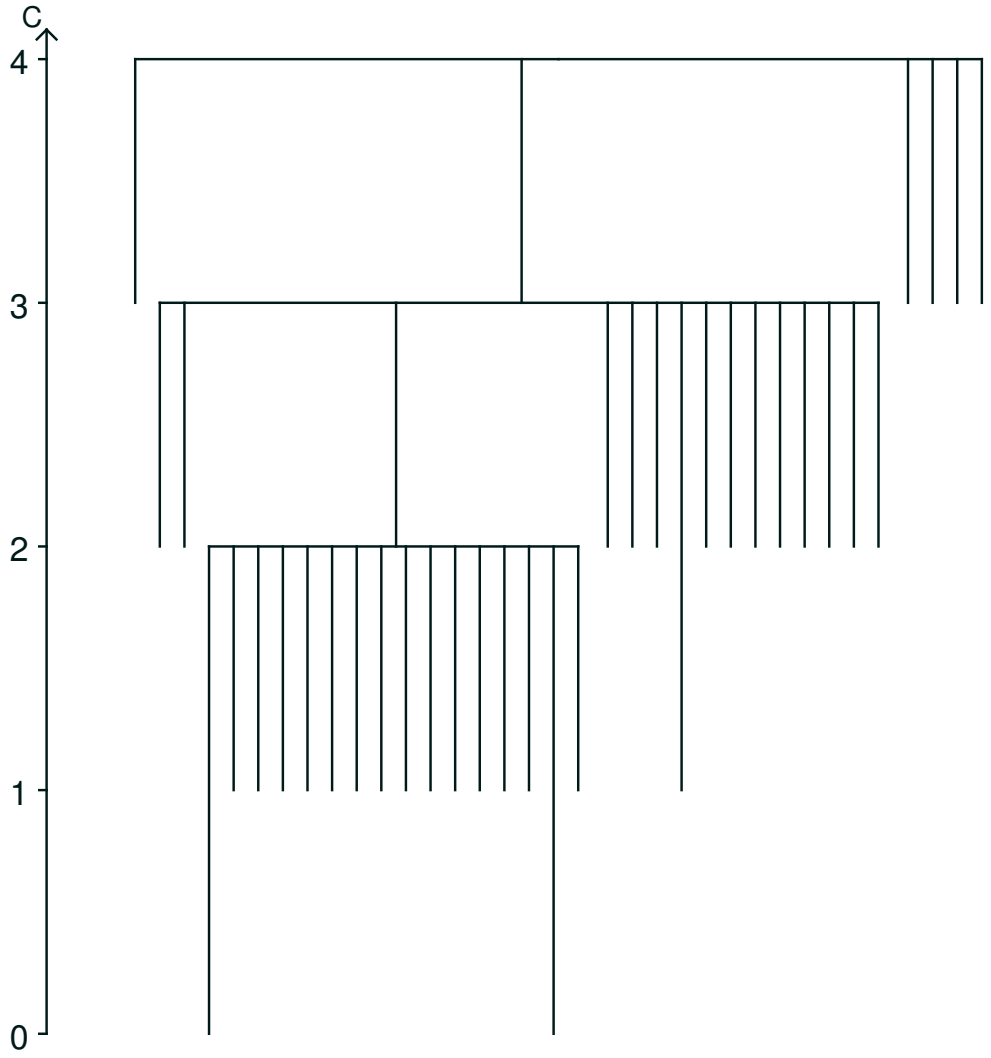
MAX-3-SAT $\alpha = M/N = 5$ $N = 30$



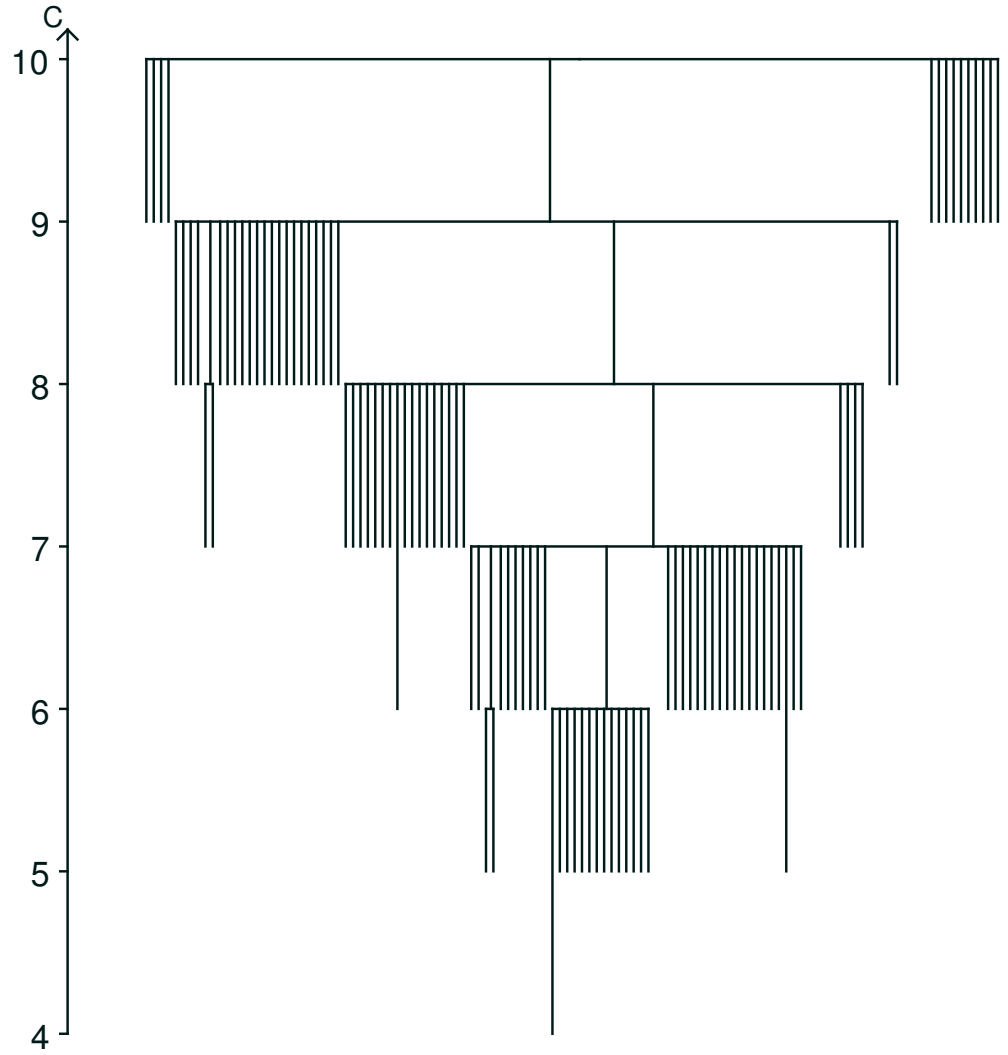
MAX-3-SAT $\alpha = M/N = 5$ $N = 40$



MAX-3-SAT $N = 40$ $\alpha = M/N = 4$



MAX-3-SAT $N = 40$ $\alpha = M/N = 6$



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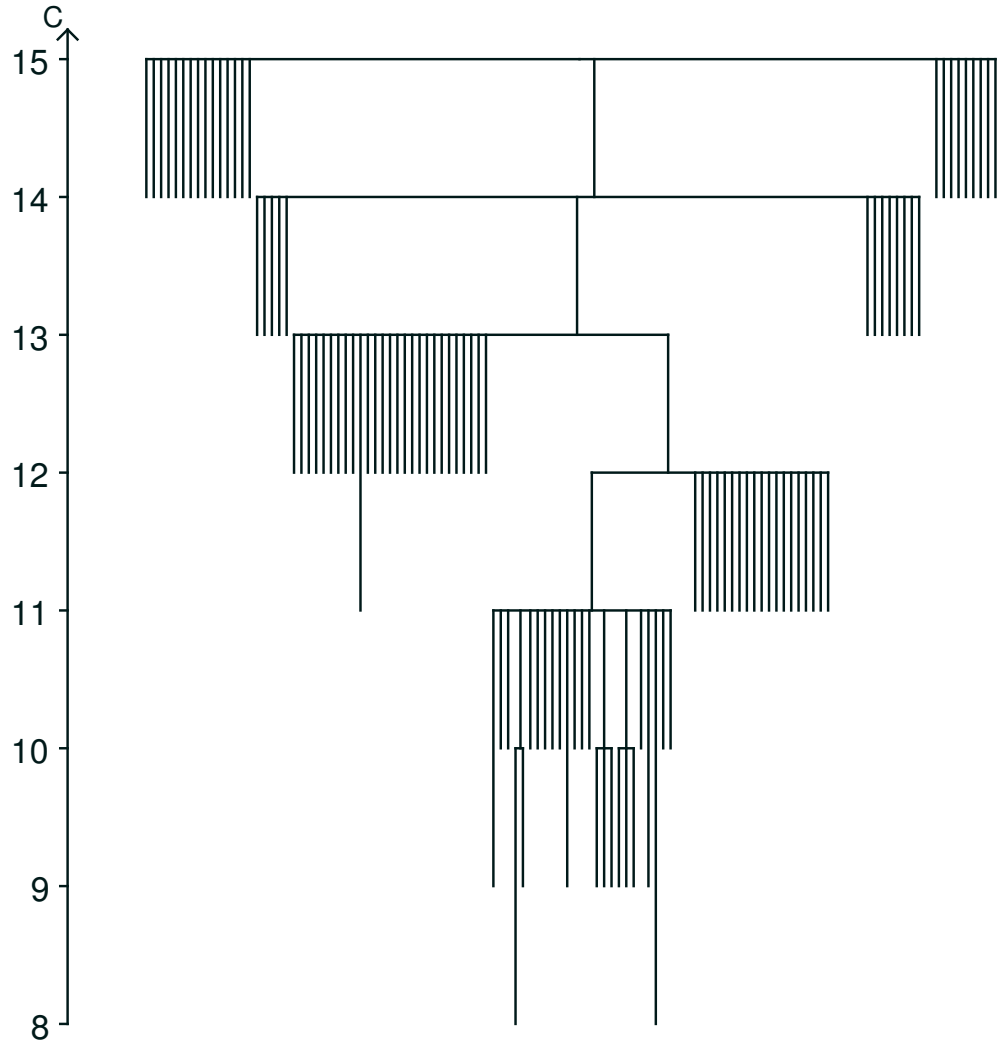

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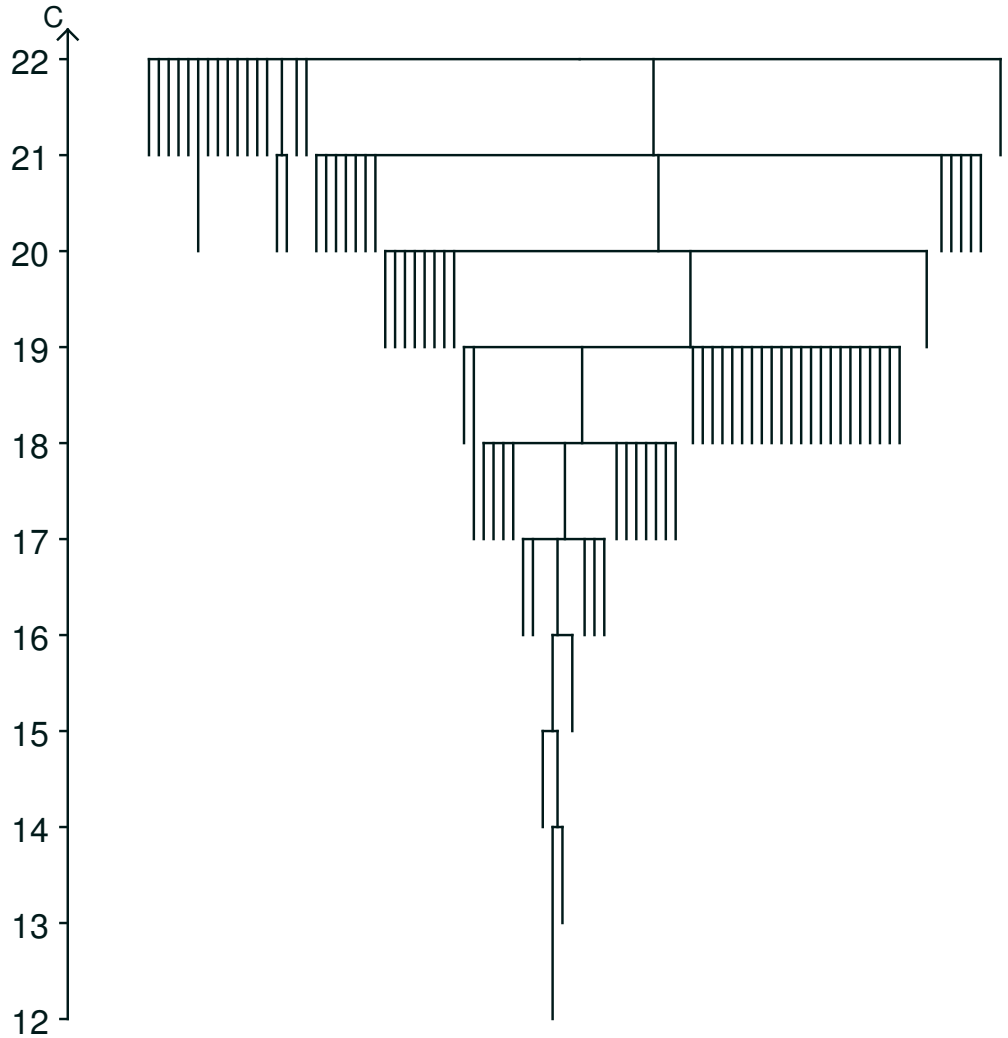
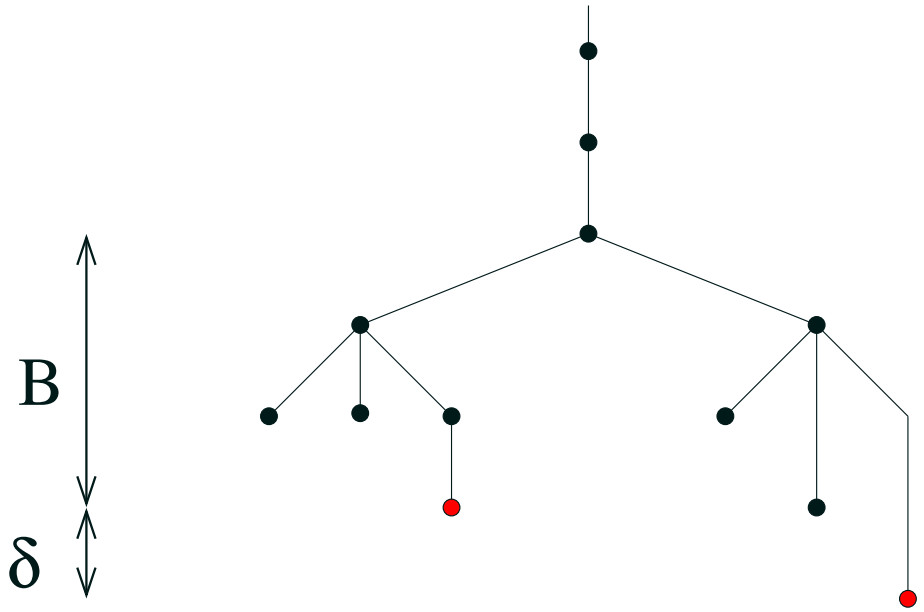


Phase Transition in Number Partitioning

- Are phase transitions evident in barrier trees?
- Studied by Stadler, Hordijk and Fontanari
- Very little evidence in shape
- Phase transition in difficulty B/δ



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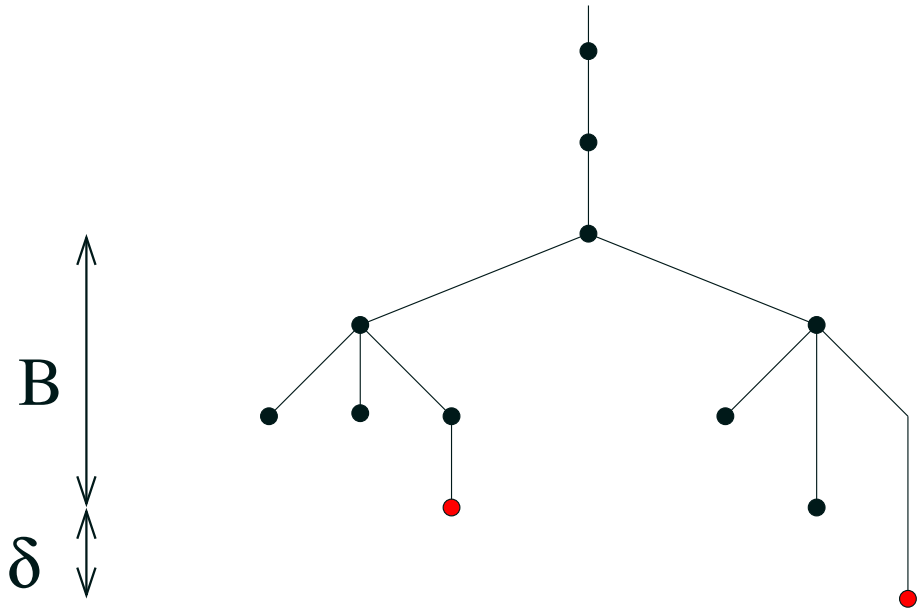

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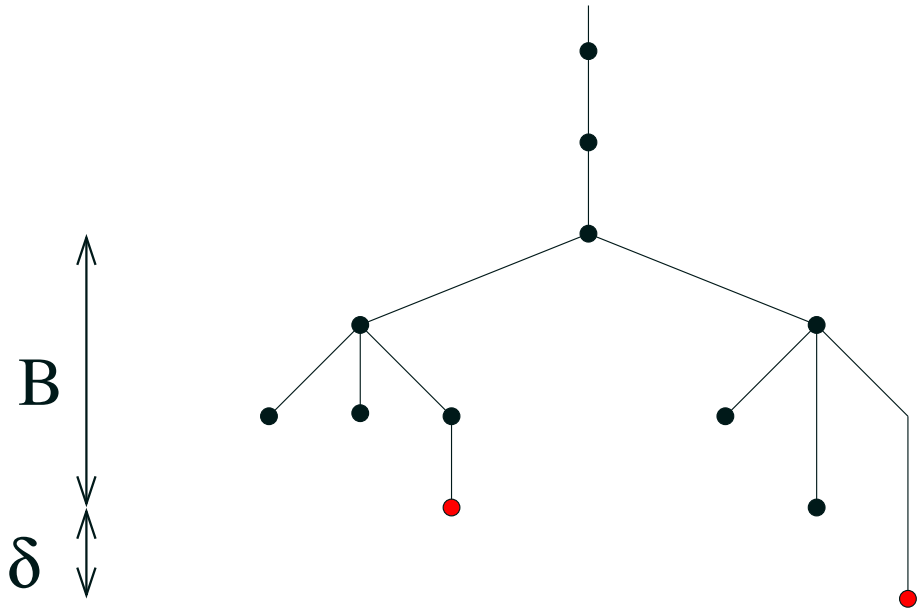

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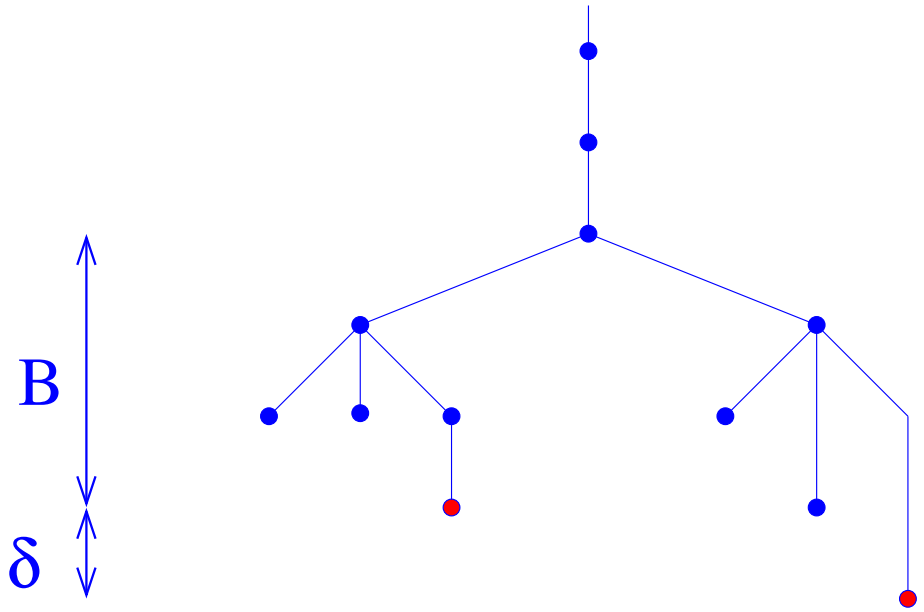

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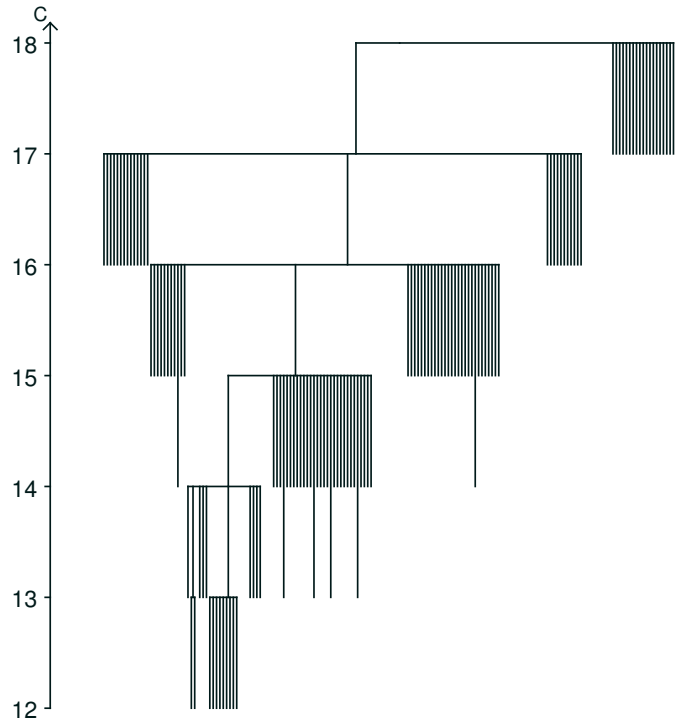

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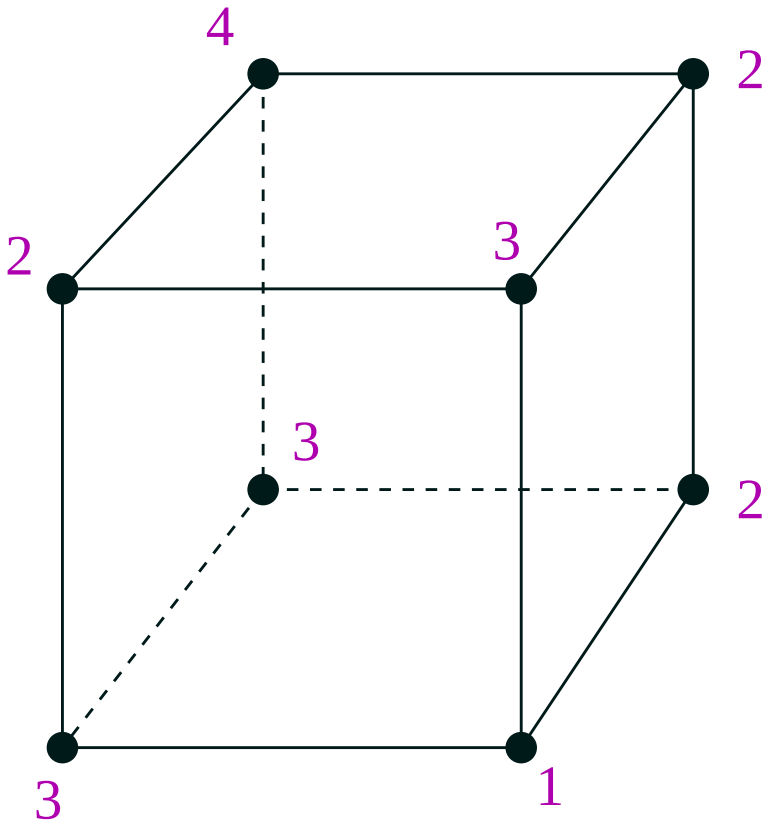

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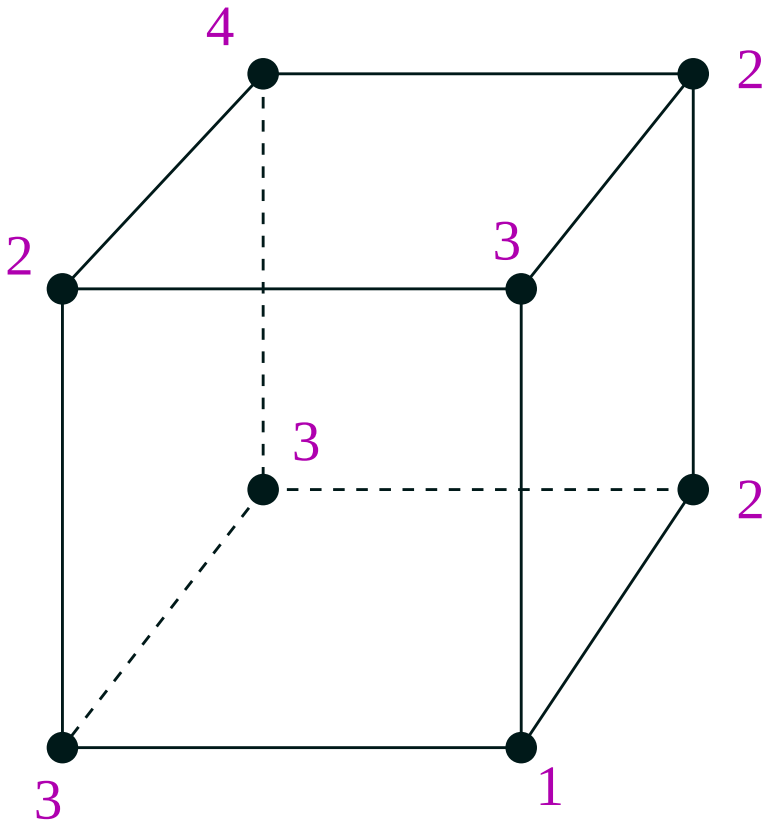

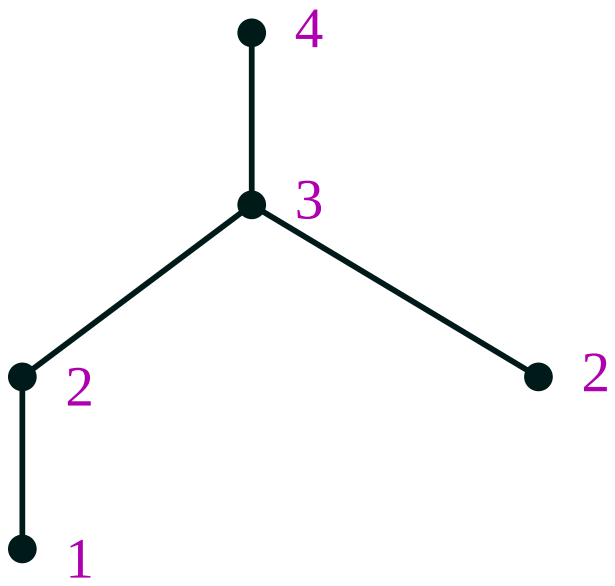

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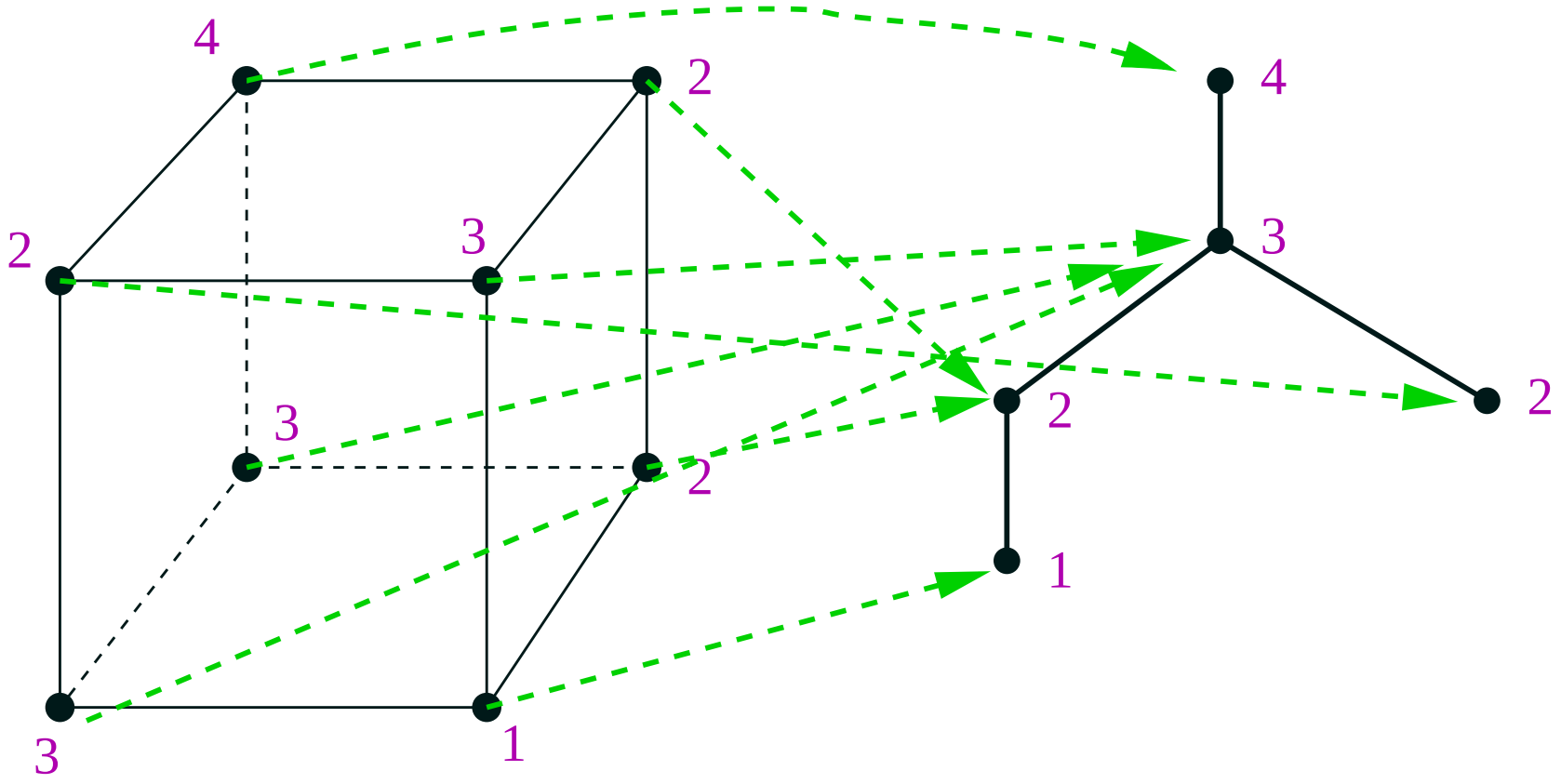

Mapping Configurations

- Every configuration is mapped to a node of the Barrier tree
- We can study statistical properties of the tree vertices
  - ⋆ number of configurations in a state
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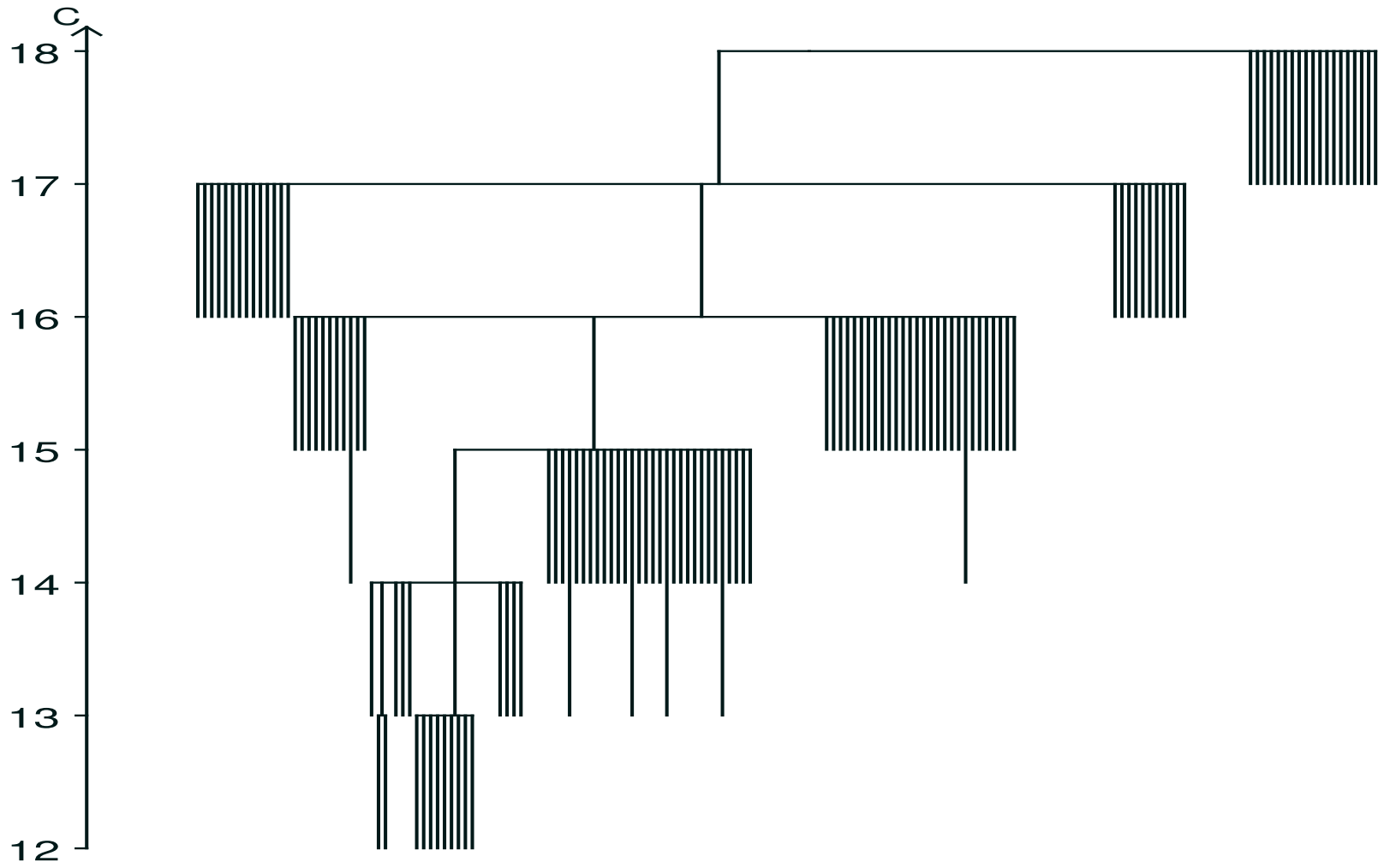
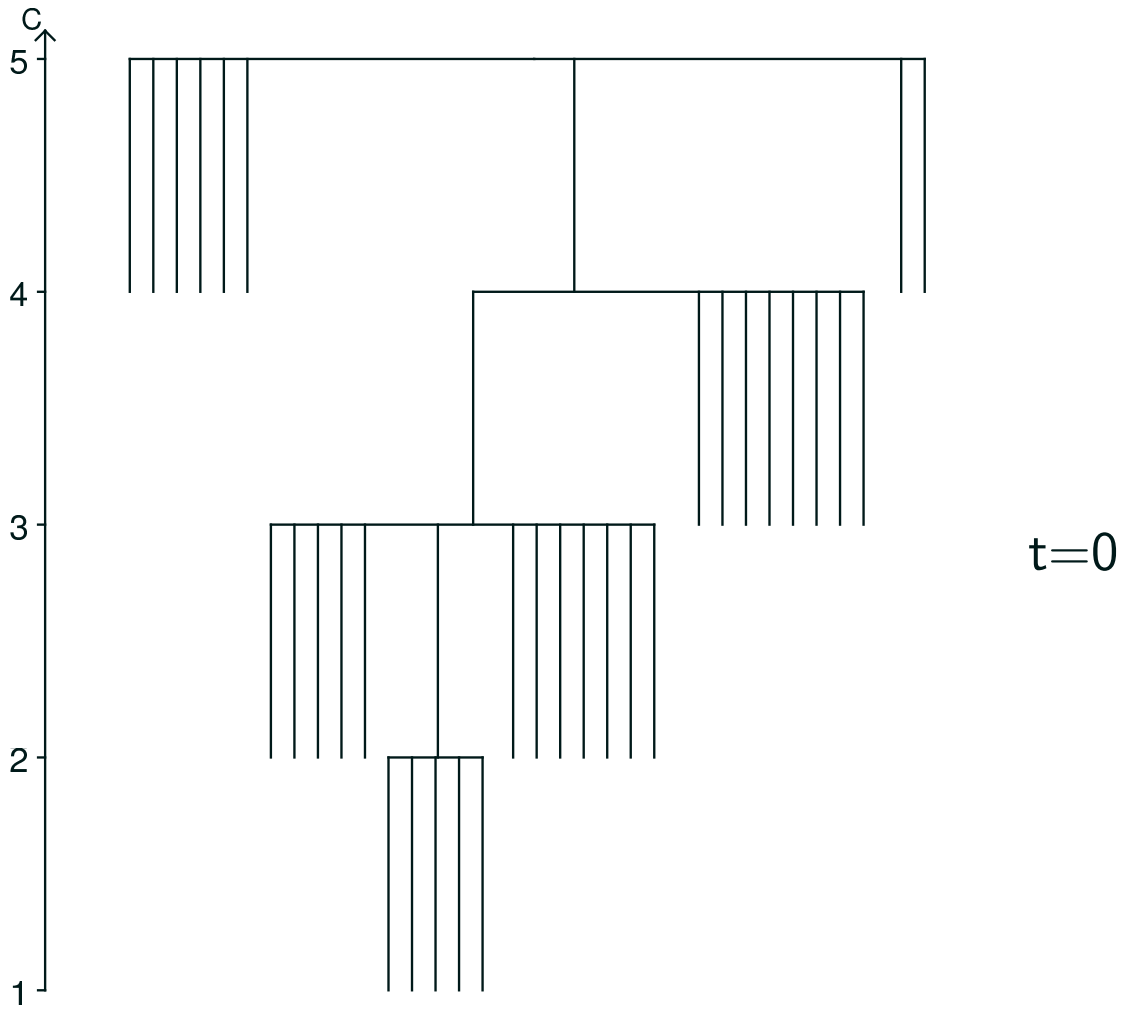


Statistics

Cost	# of configs	# of minima	Mean basin size	# minima depth > 1	% configs local minima	# of saddle points	% descents runs
16	210560	25	2.44	0	0.029	1	2.06
15	46518	37	4.29	0	0.34	1	9.09
14	8336	28	3.93	2	1.3	1	18.04
13	1041	12	10.92	4	12.6	2	18.45
12	47	11	4.27	0	100.0	0	50.71

Simulated Annealing 40 Variables



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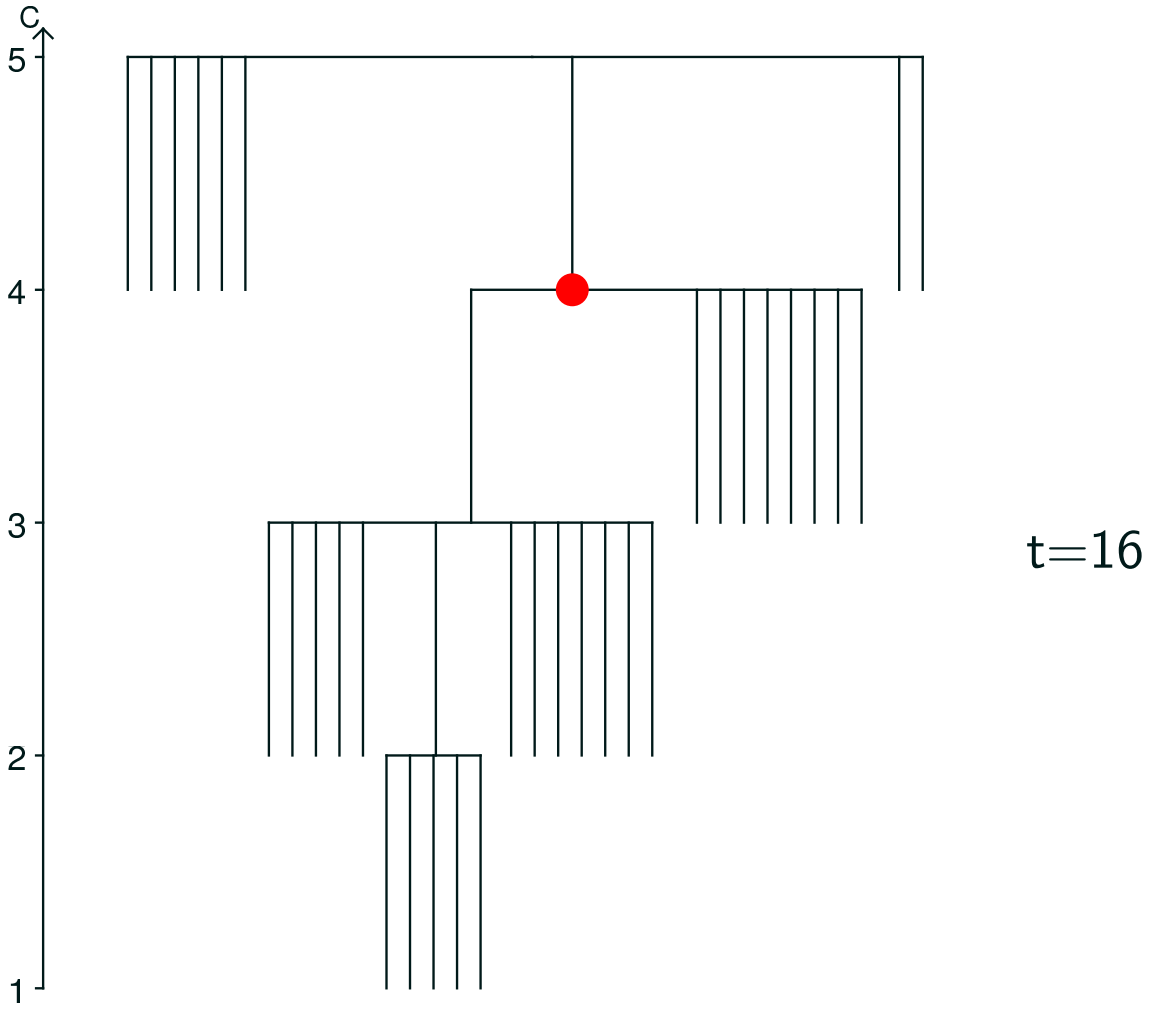

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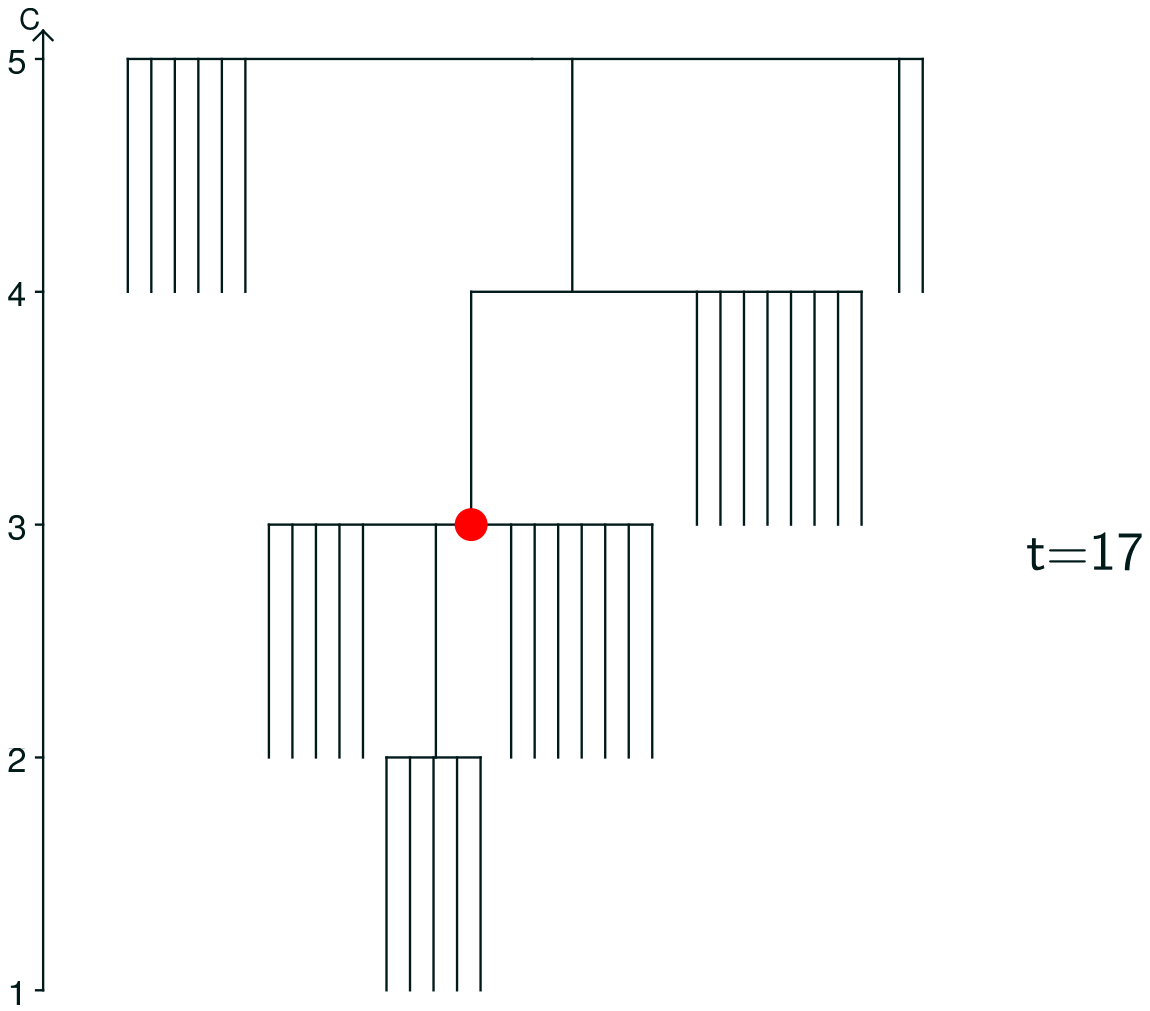

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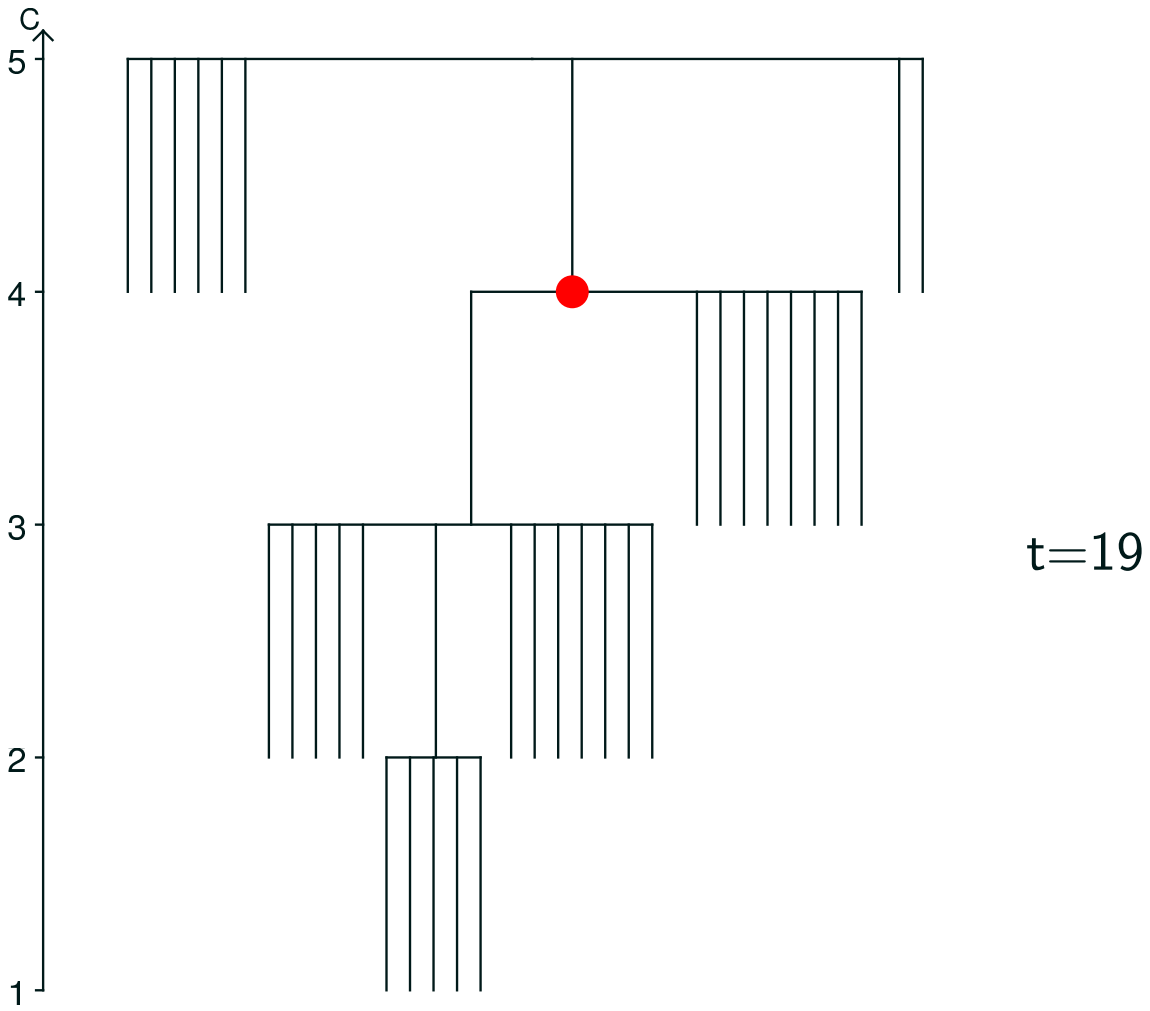

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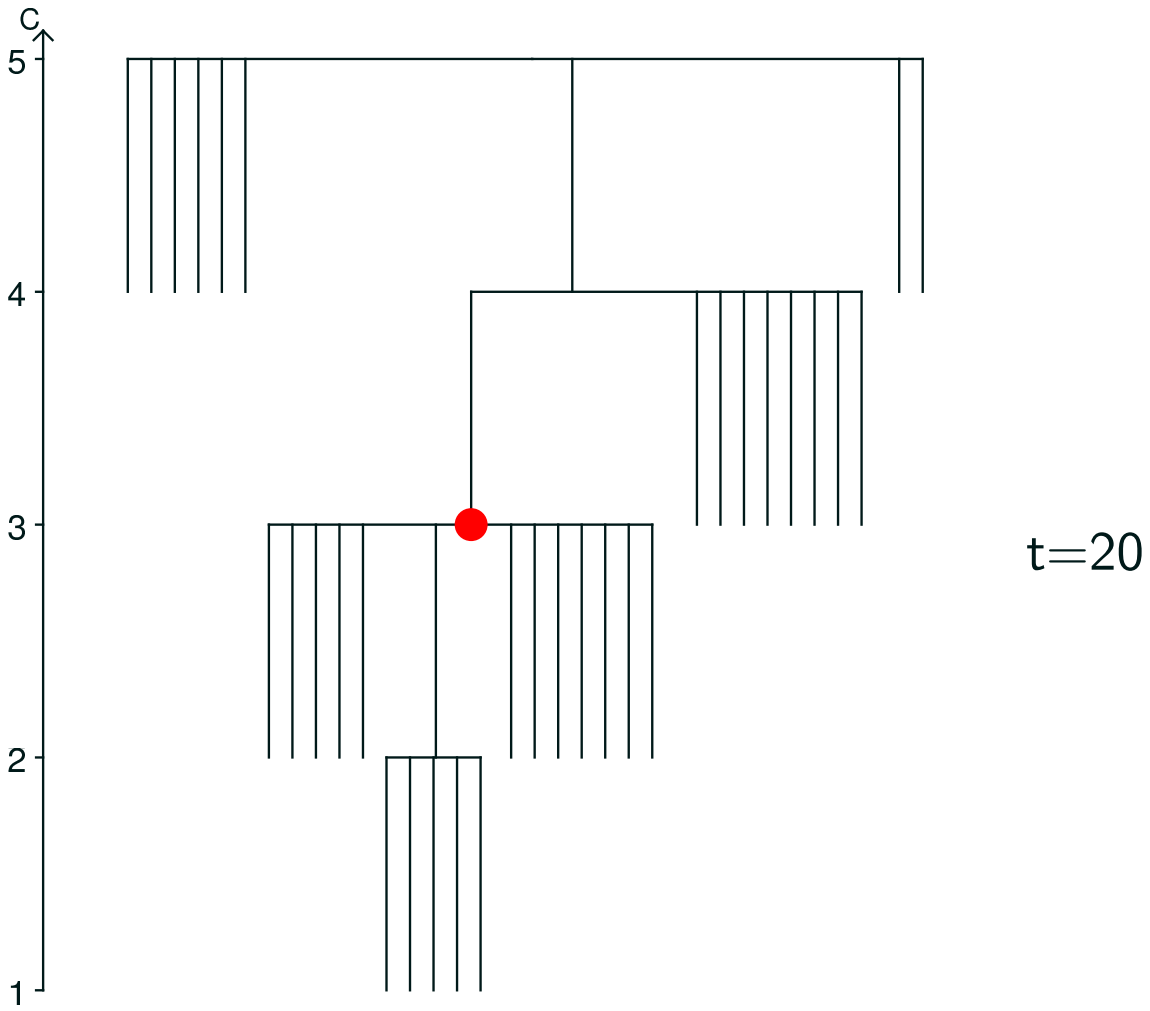

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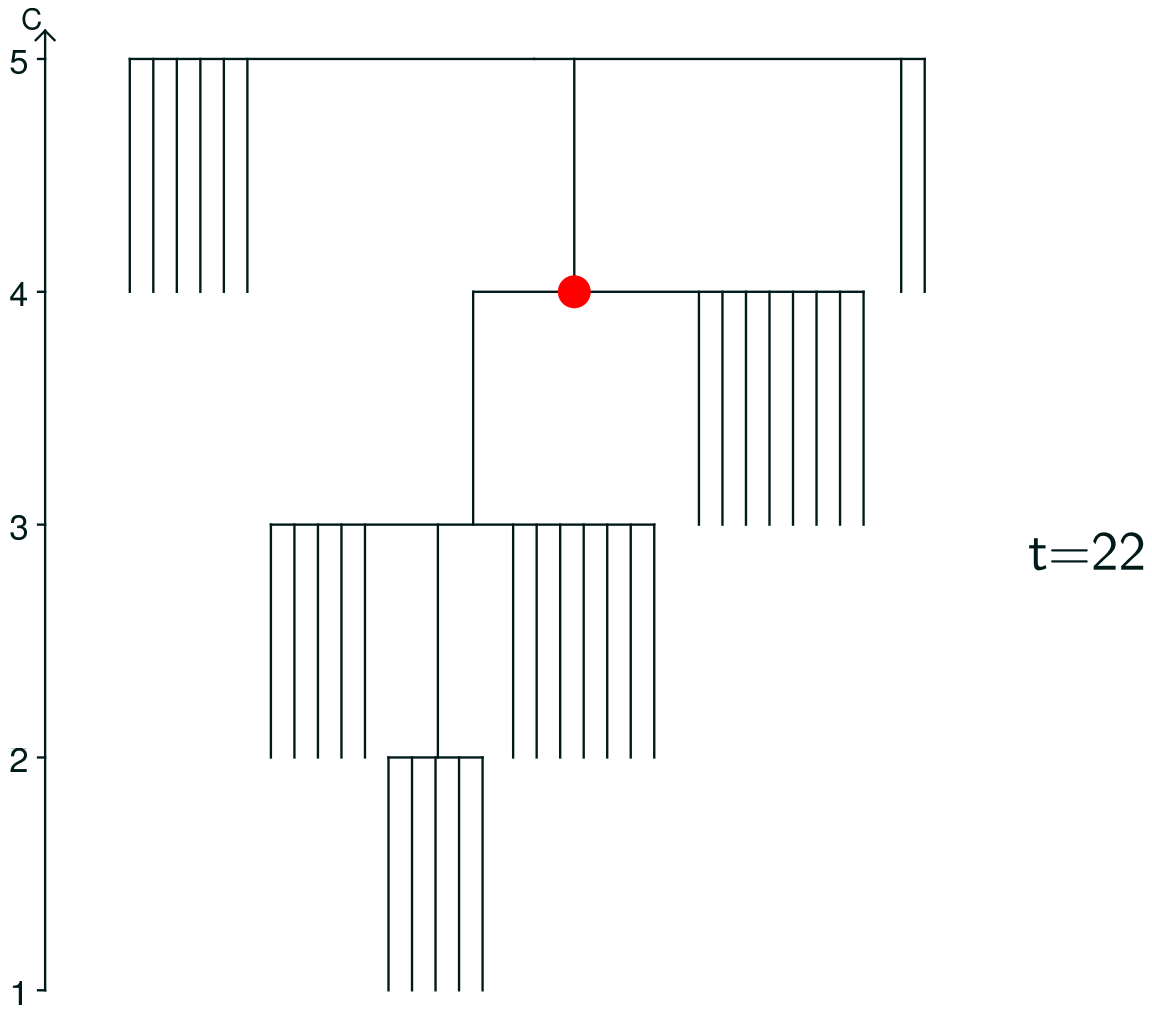

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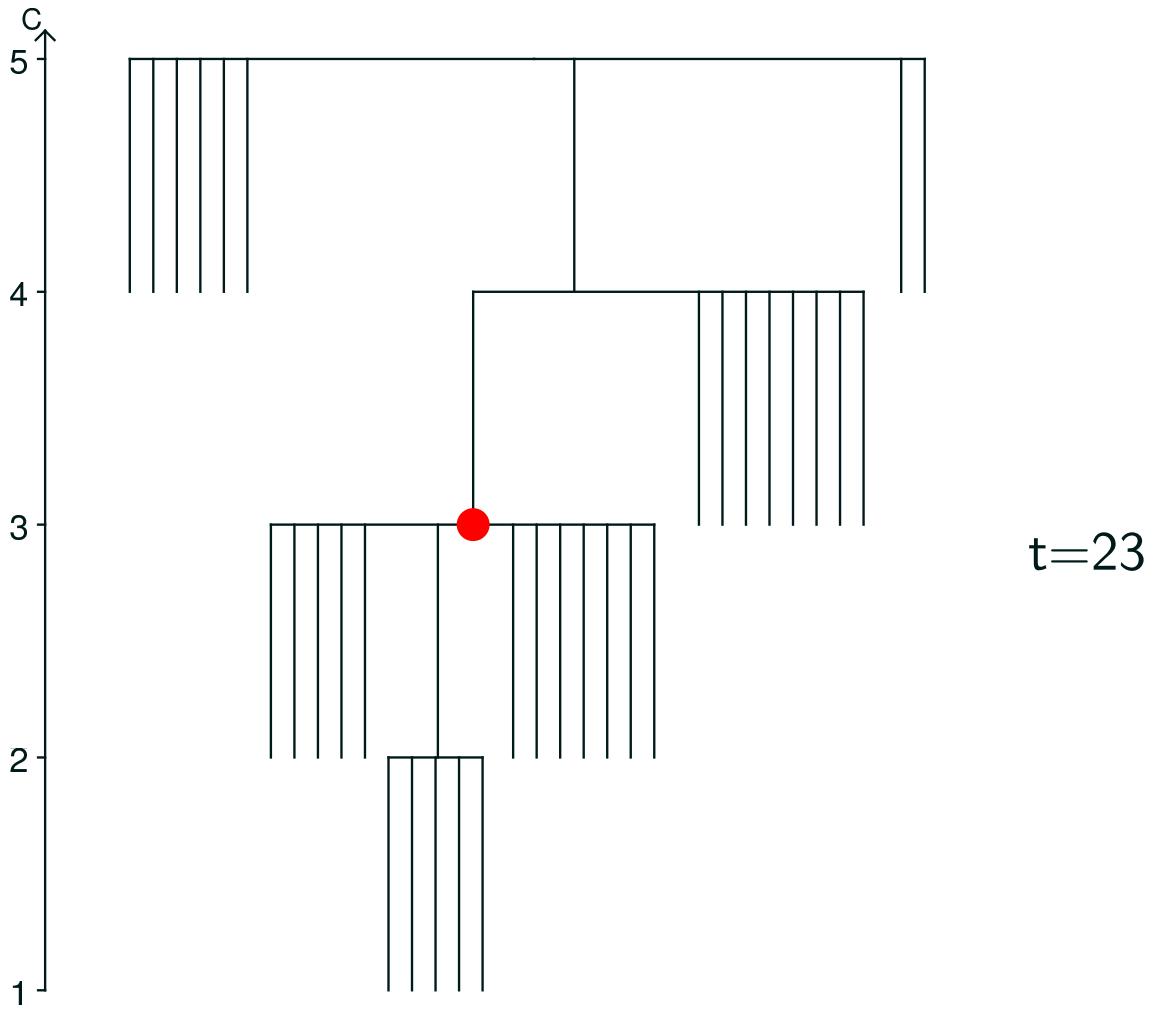

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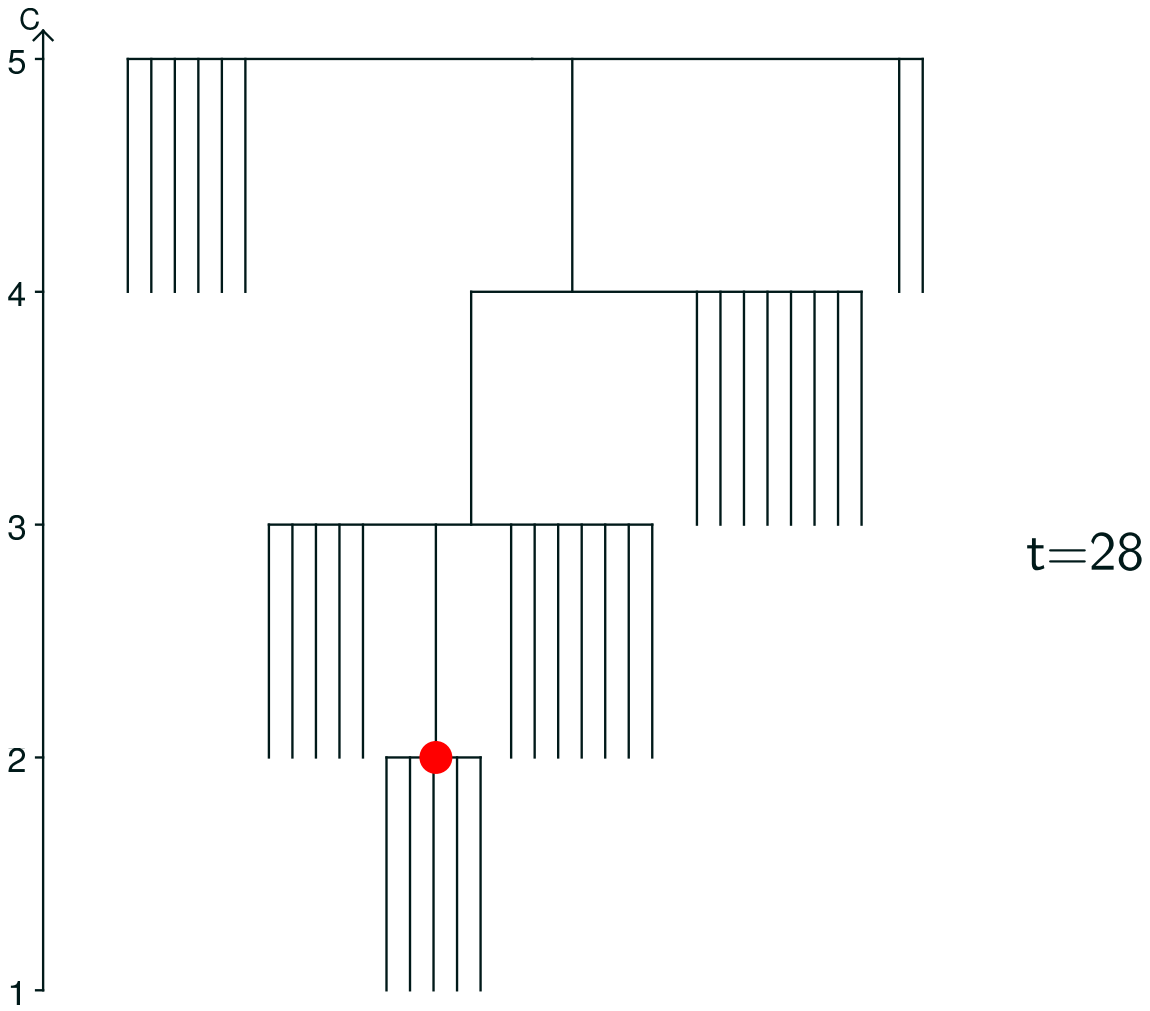

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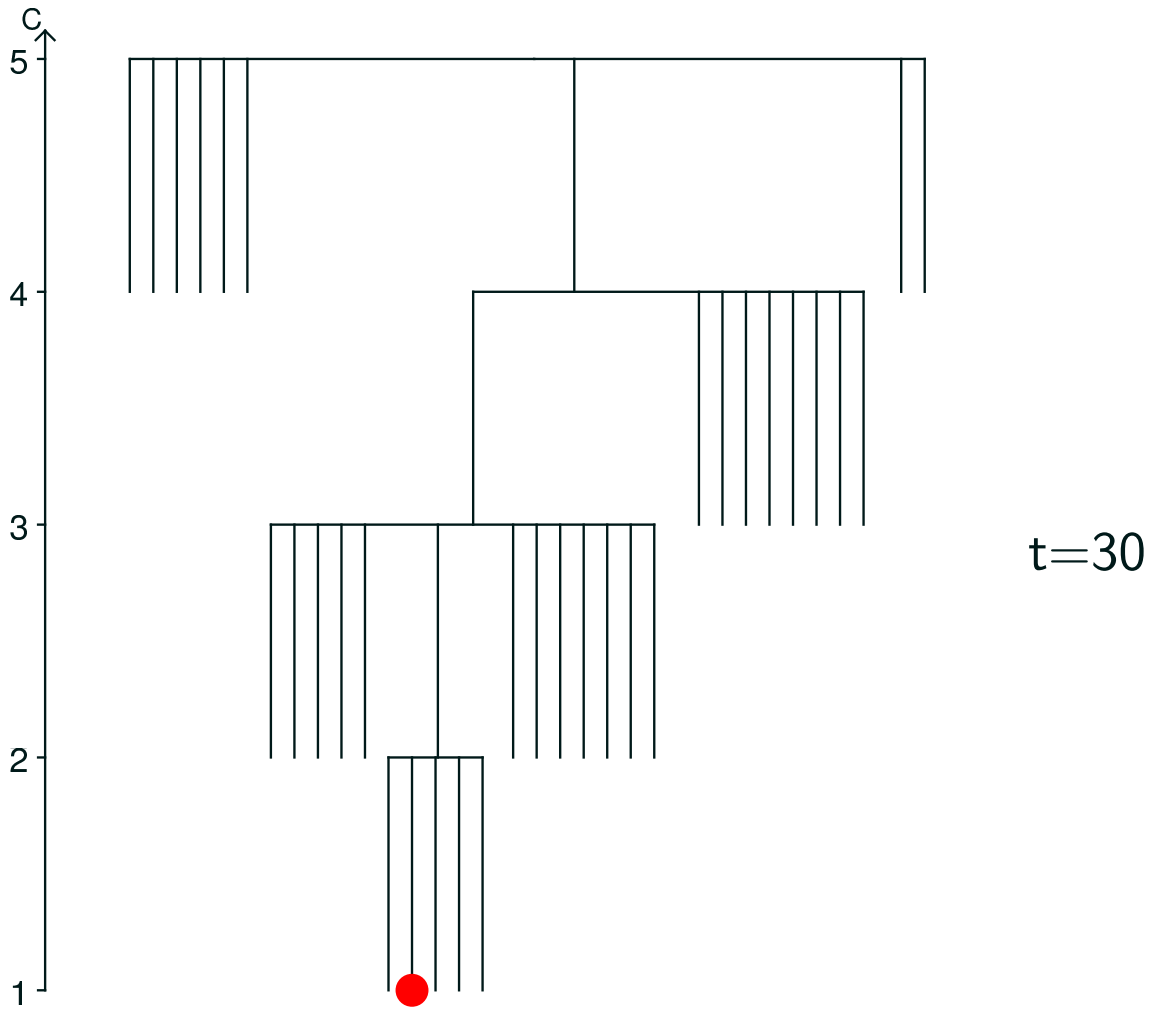

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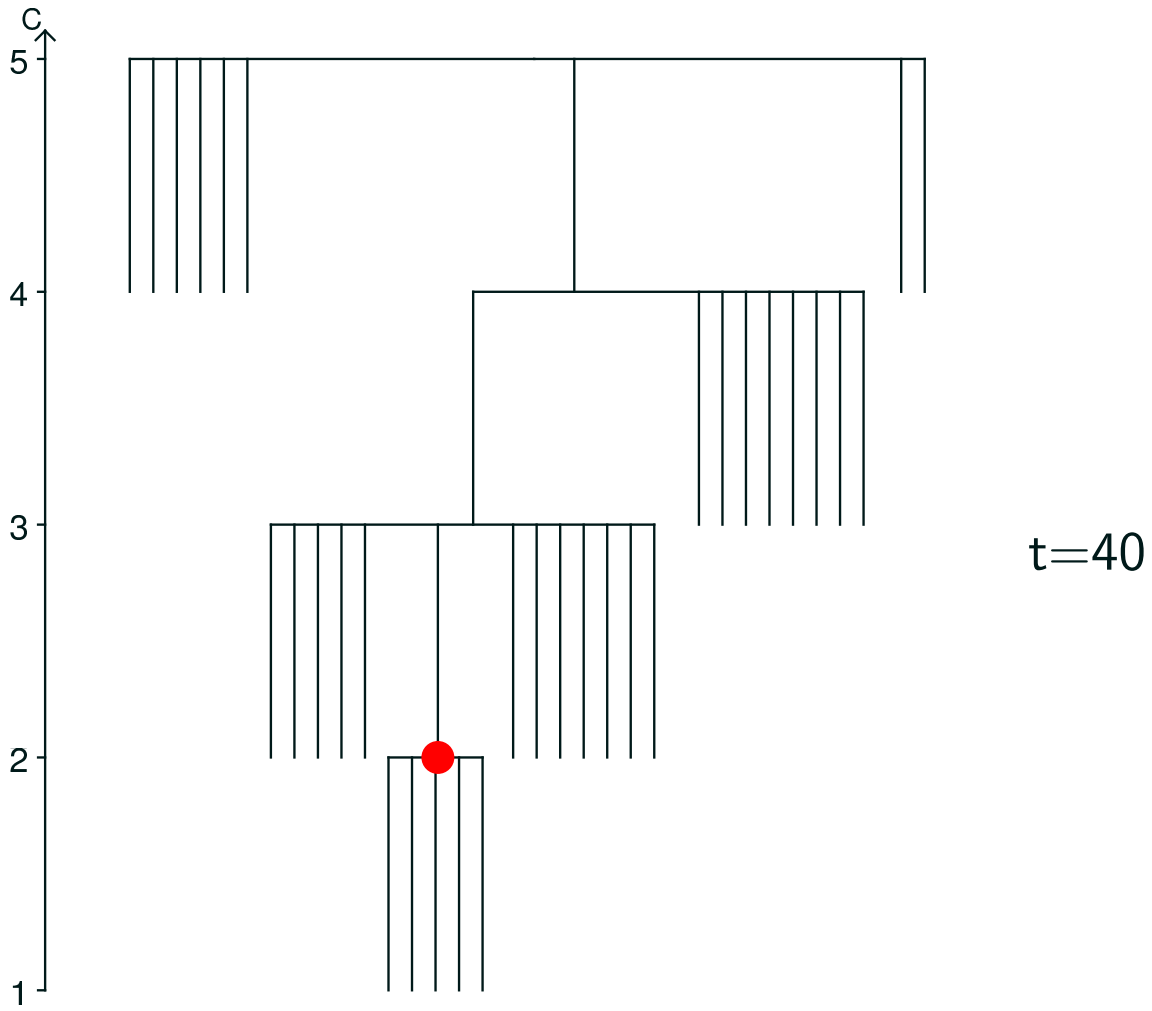

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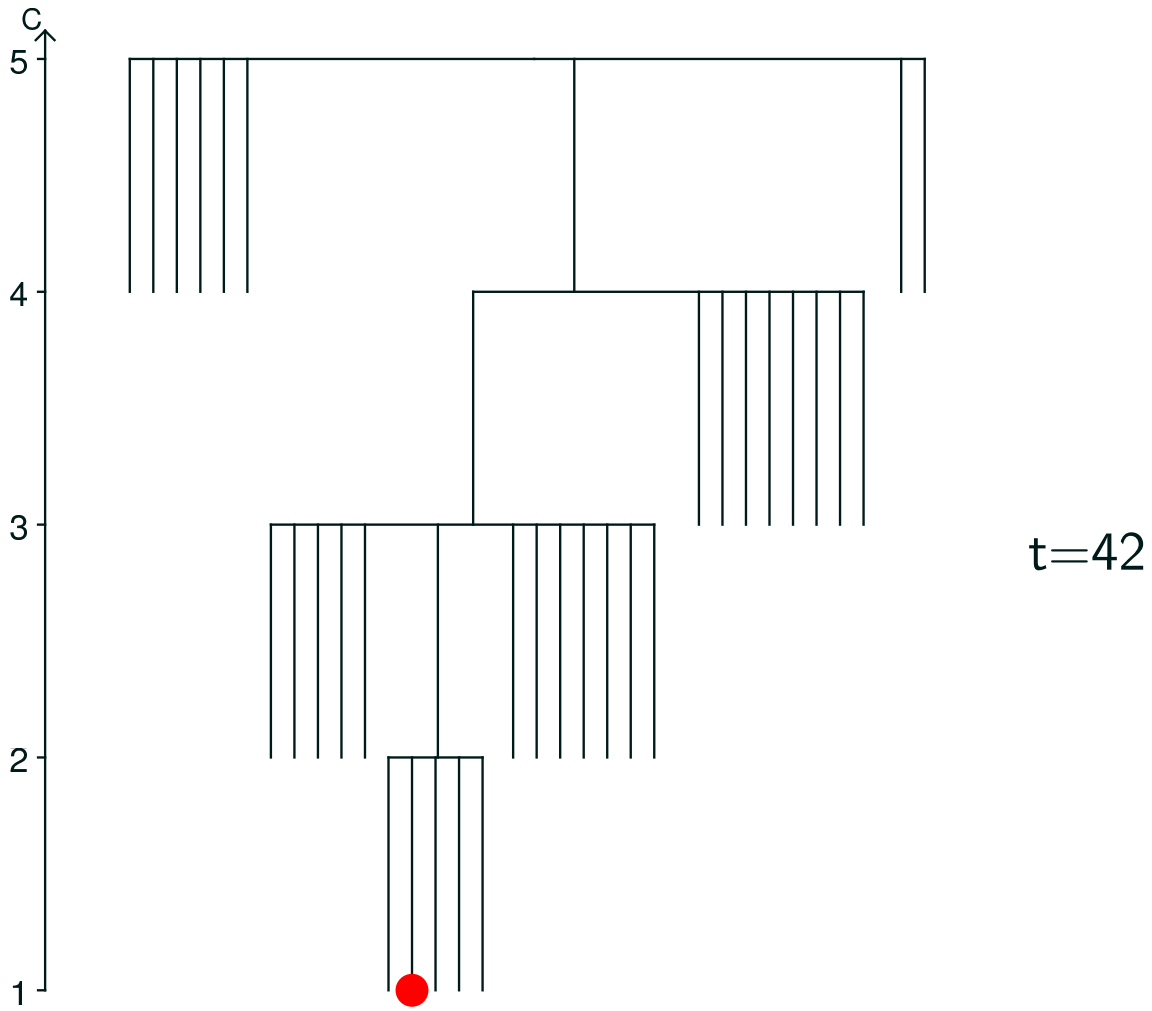
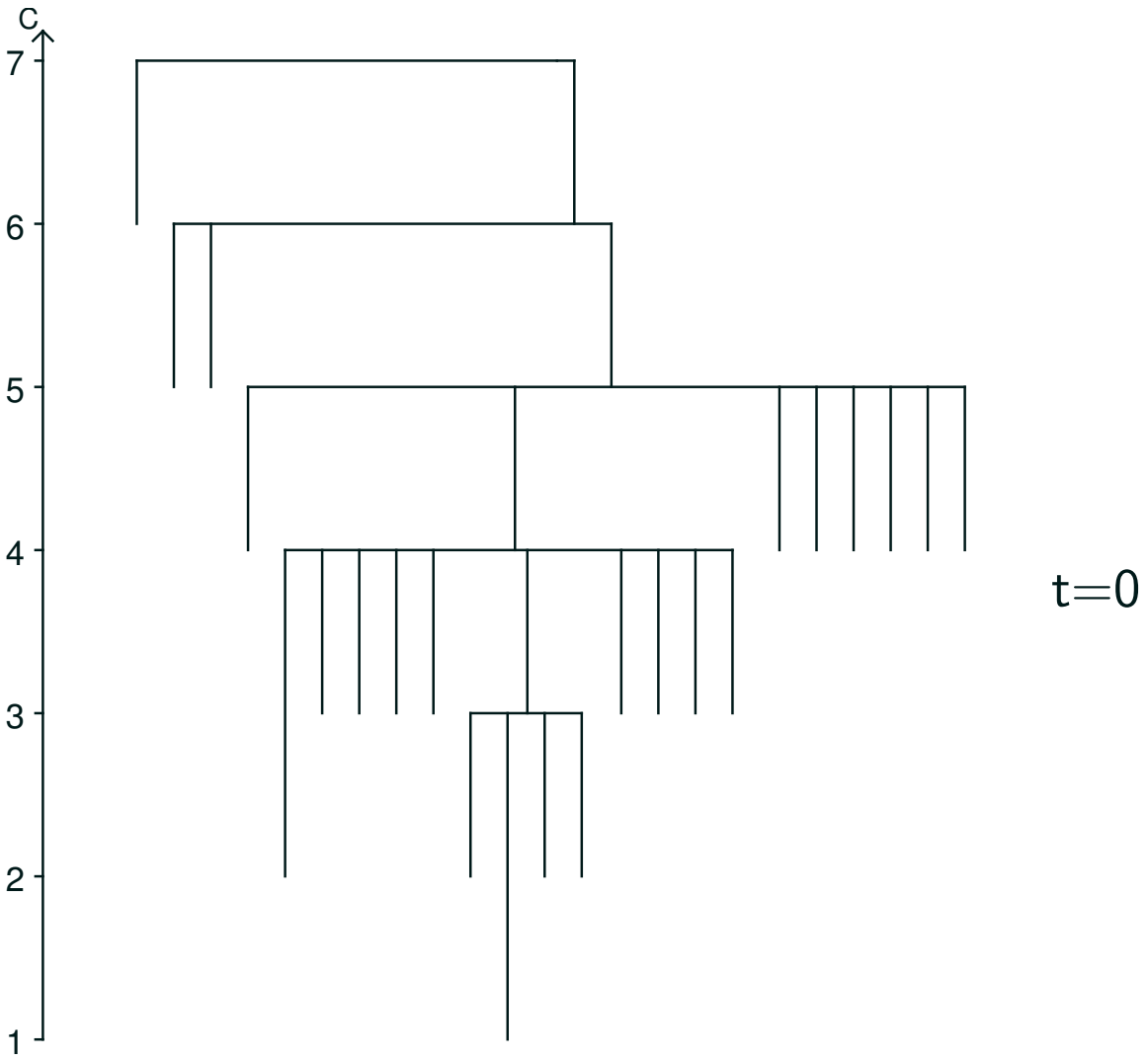


Genetic Algorithms 30 Variables



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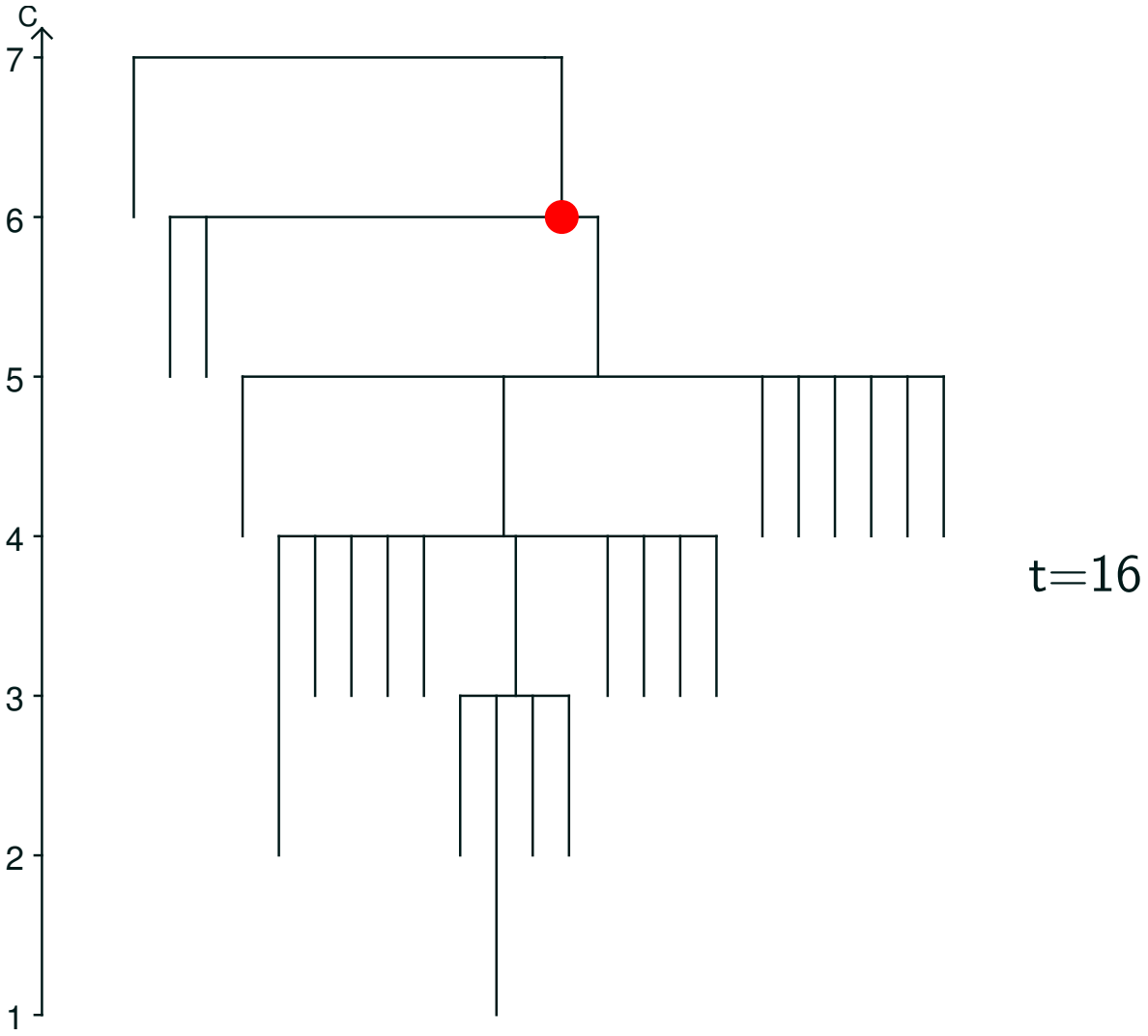

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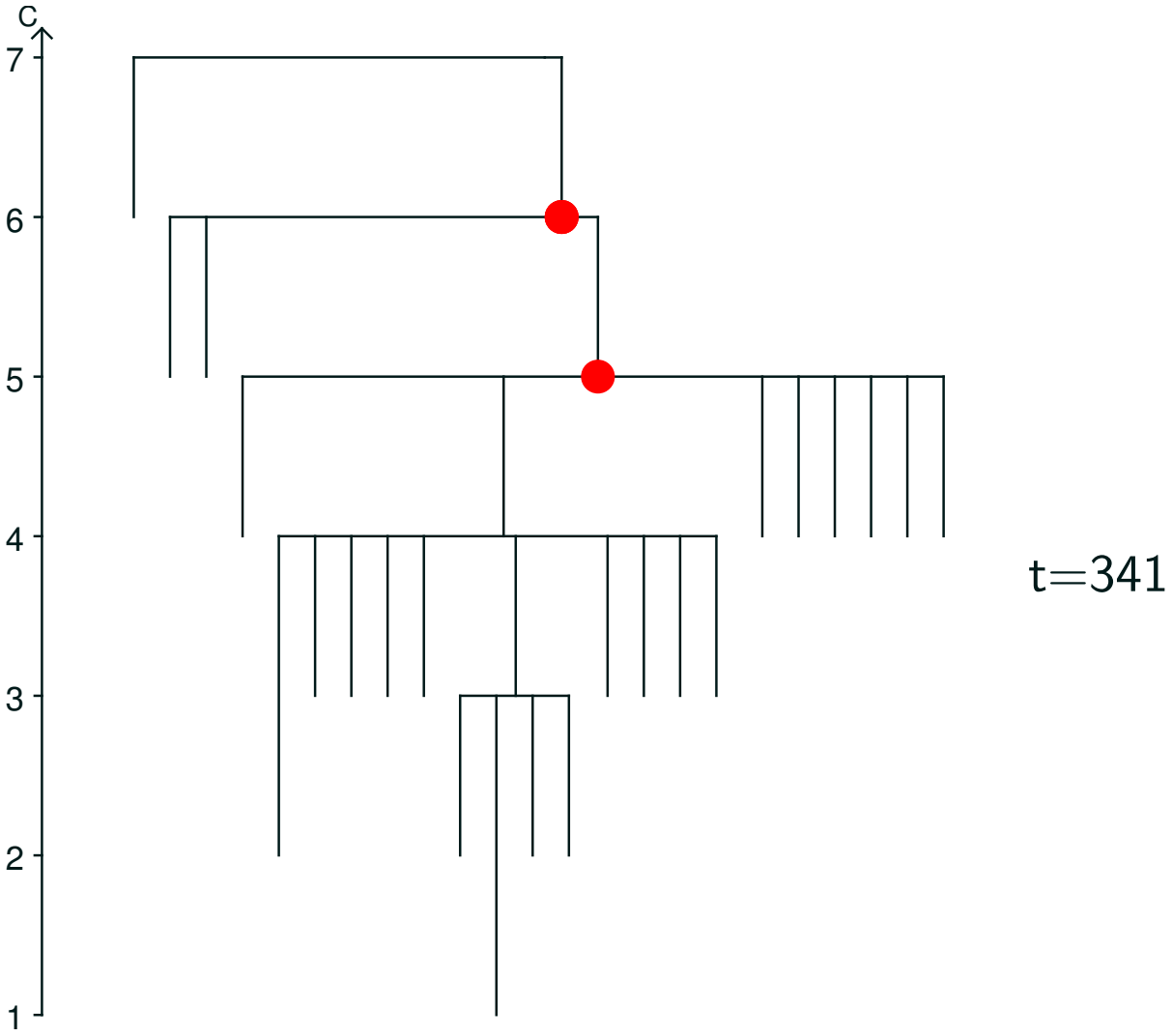

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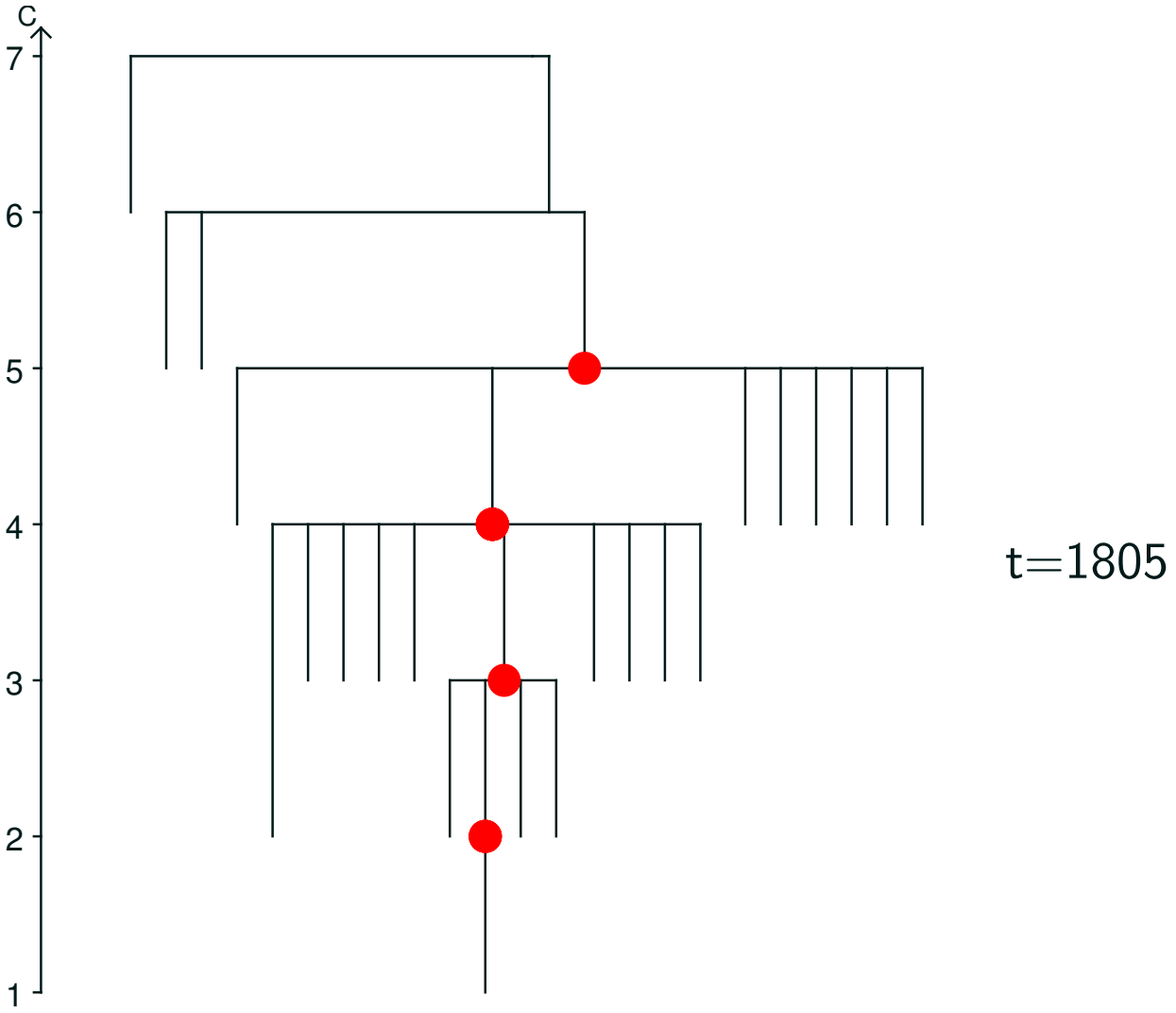

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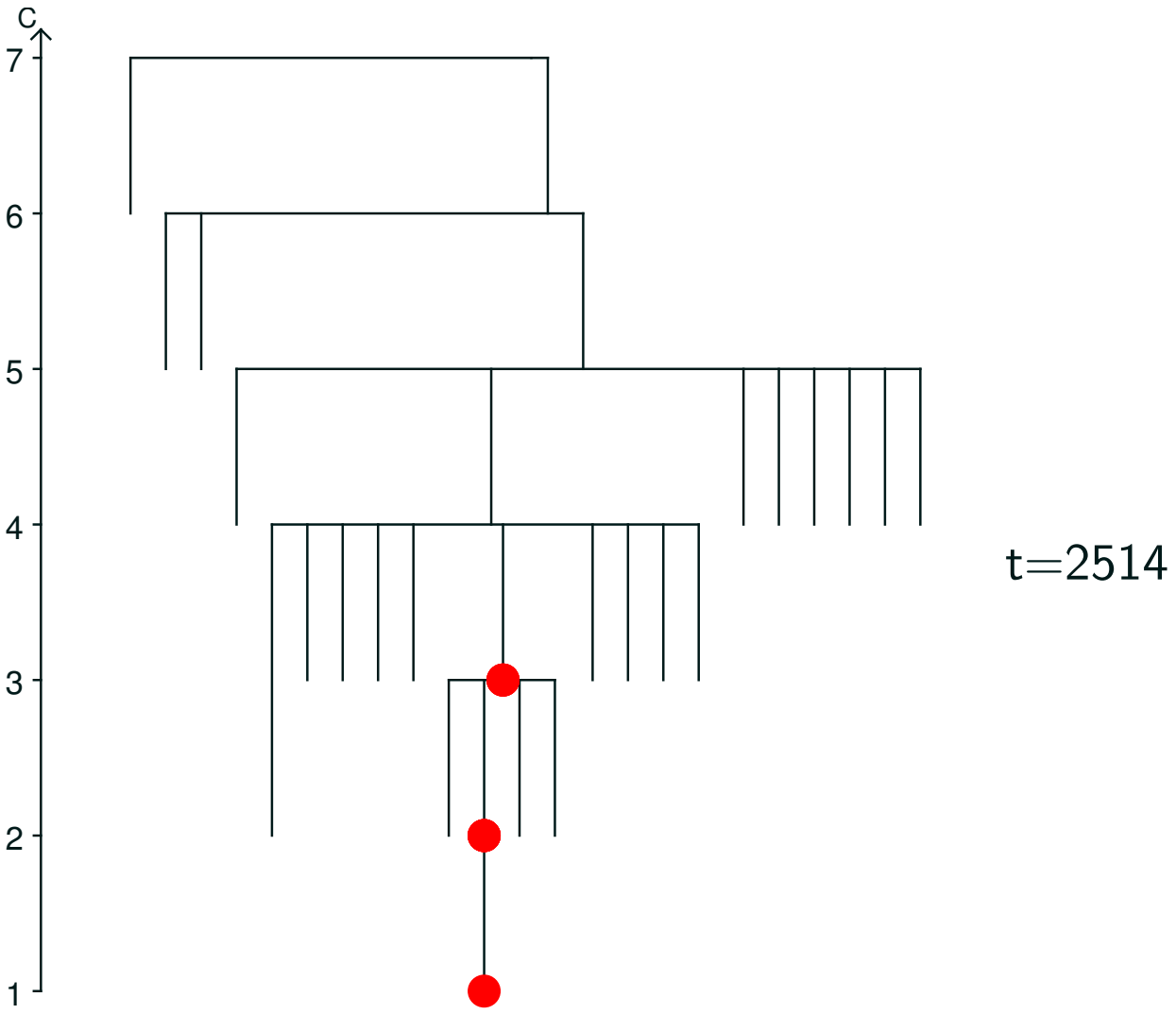
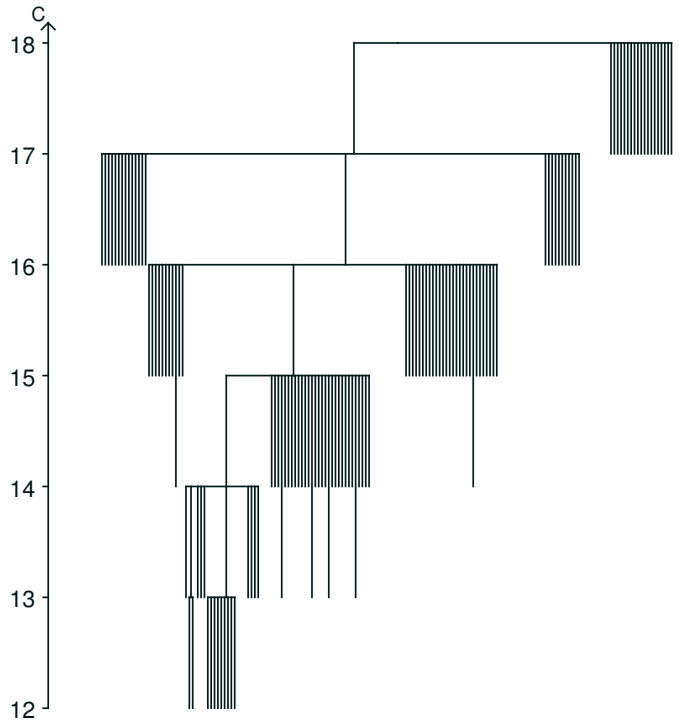


Outline

1. Optimisation Problems
2. Cost Landscapes
3. Barrier Trees
4. Example Instances
5. Mapping Configurations
6. Modelling the Problem



Modelling Optimisation Problems

- Model problems by amalgamating configurations
- Each node of on the barrier tree is a state
- Initial occupancy given by number of configurations in state
- Transition probabilities proportional to number of neighbouring pairs
- This is an approximation!
- Model has same structure of local minima and barriers as true problem

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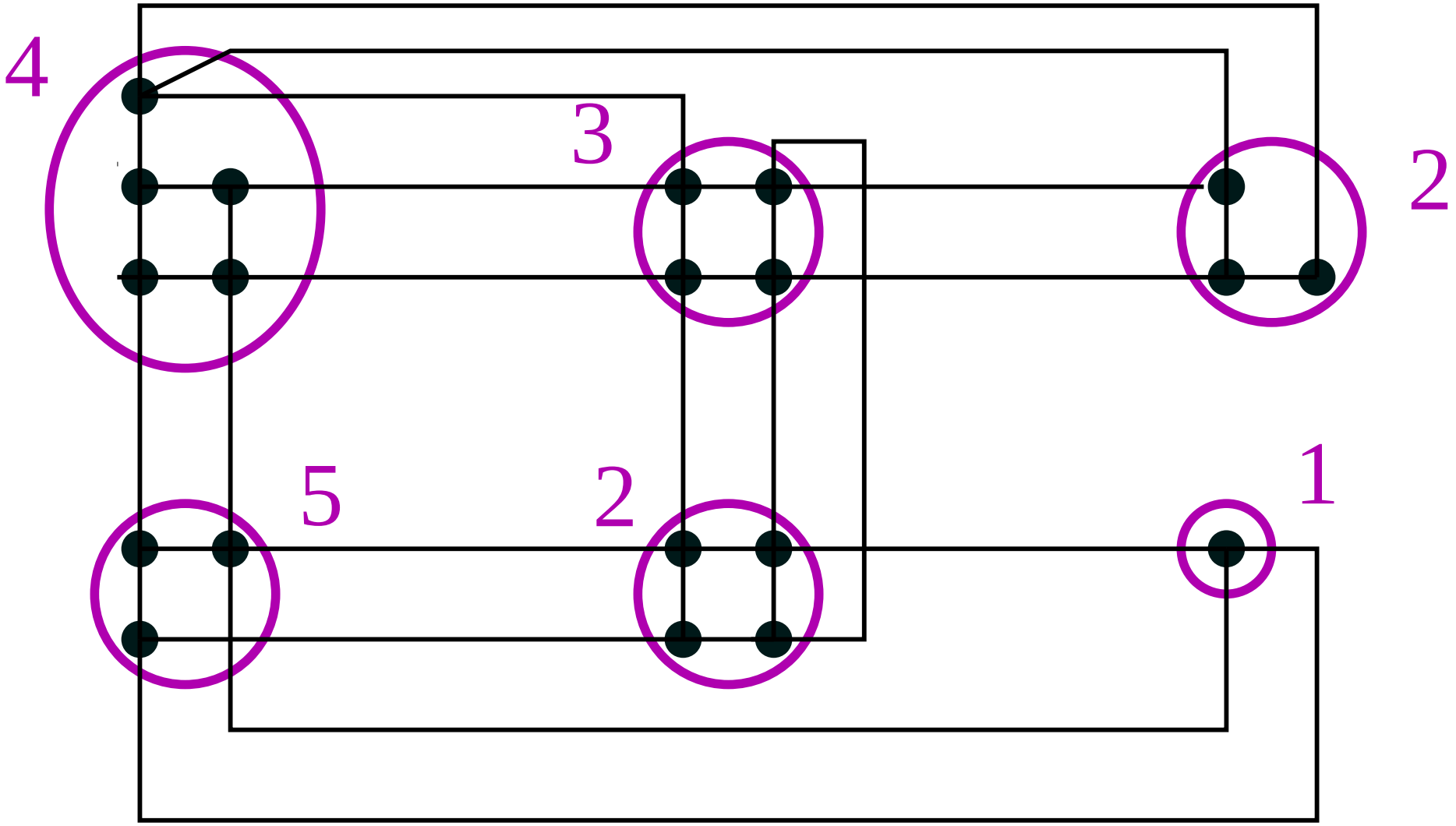
Schematic of Model Problem



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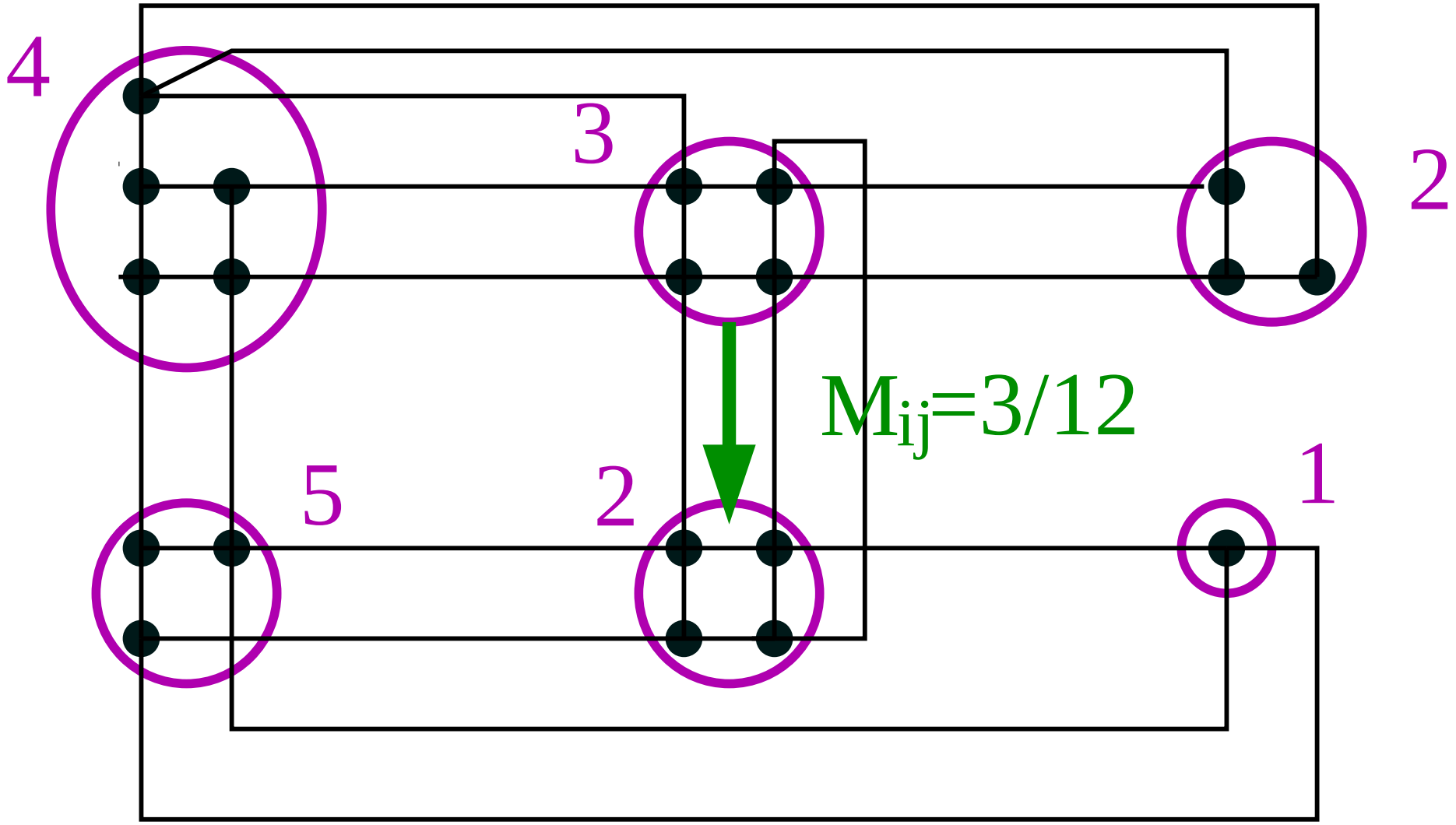
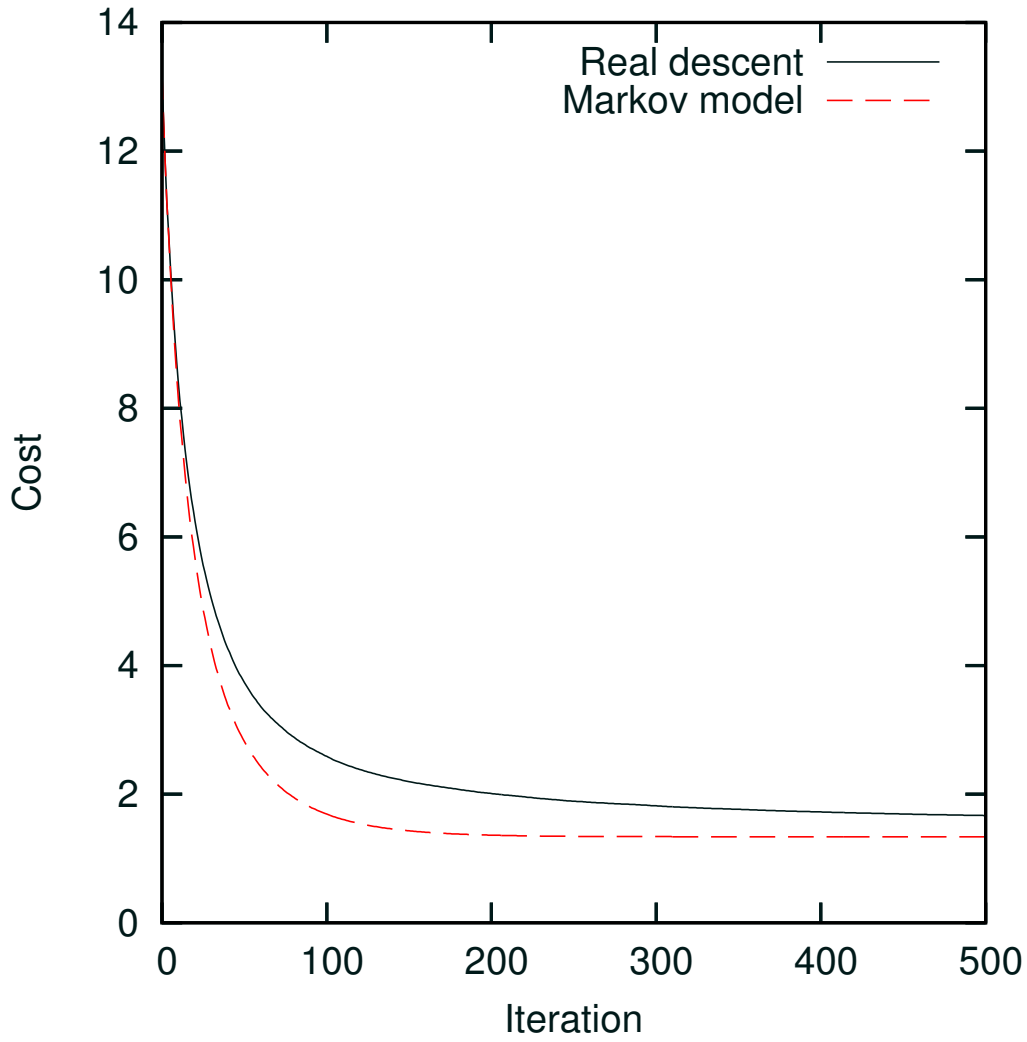
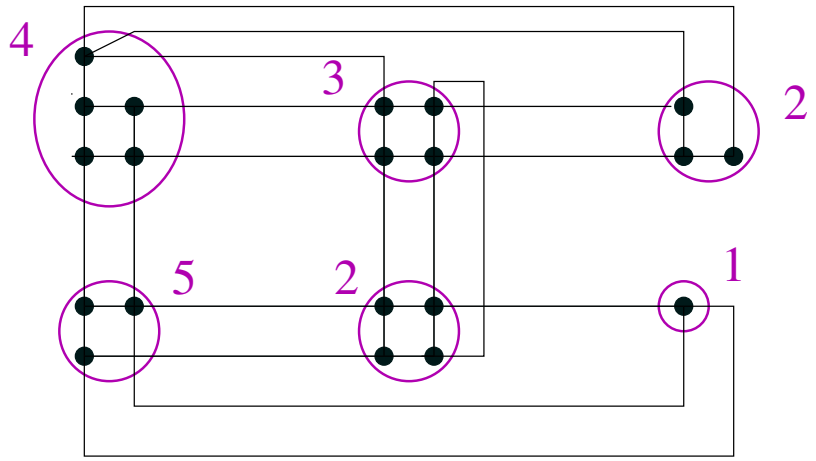


Descent: Max-3-Sat $N = 20$, $\alpha = 6$



Comparison with True Problem

- Same qualitative behaviour
- Dynamics is slower—dynamics within state is not captured
- Model problems are systematically easier
- Configurations in state are not searched equally often



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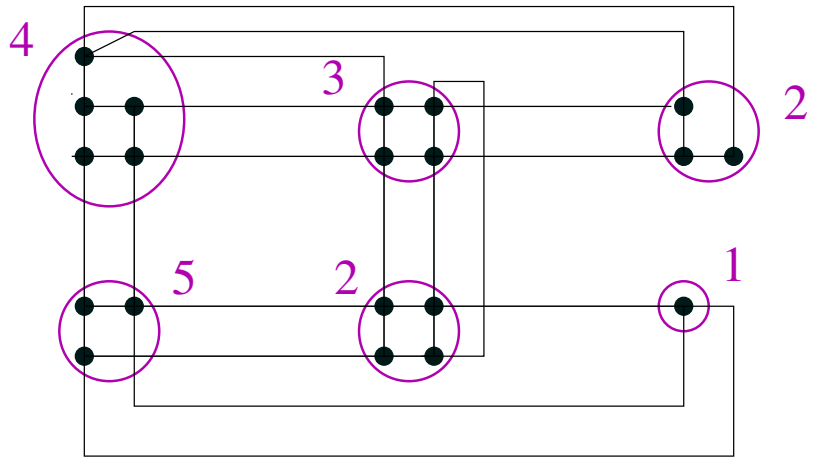

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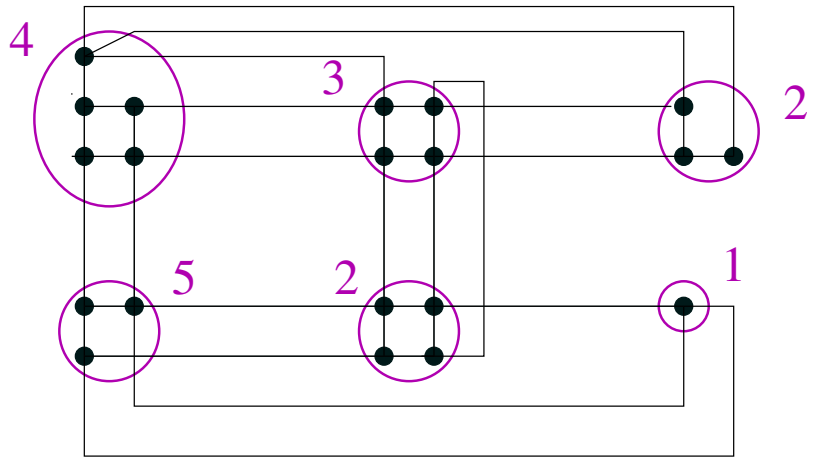

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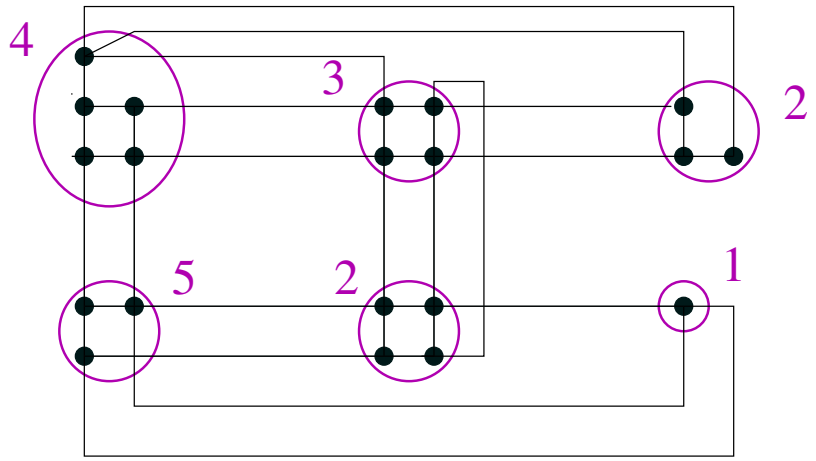

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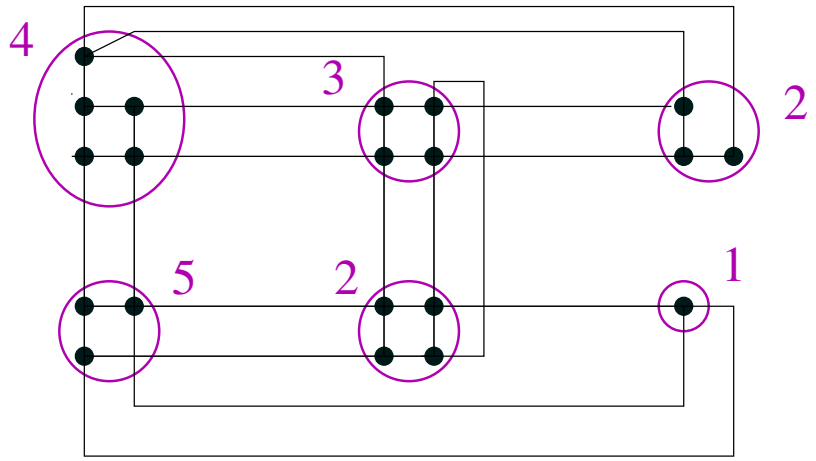
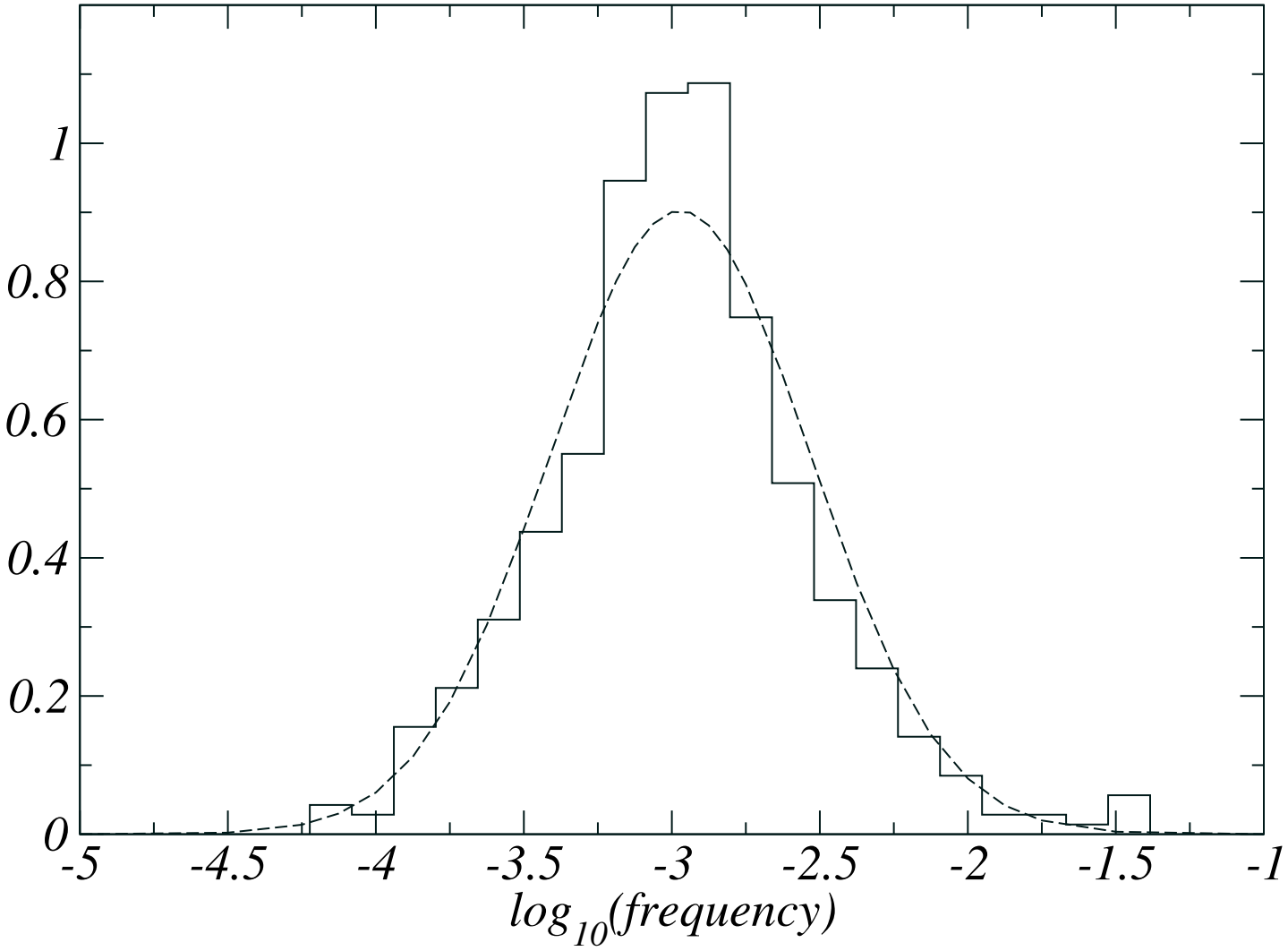


Frequency of Visiting Configurations



Configuration in a saddle-point level-connected set

Markov Models

- Many Heuristic search algorithms can be modelled as Markov processes

$$\boldsymbol{p}(t) = \mathbf{W}(t)\boldsymbol{p}(t-1)$$

- $\mathbf{W}(t)$ transition matrix
- $\mathbf{W}(t)$ depends on the connectivity matrix $\mathbf{M}$ and the heuristic
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Optimal Schedules

- We can compute optimum annealing schedule for the model analytically—has been studied previously on very small real problems
- Schedule depends on optimisation criteria
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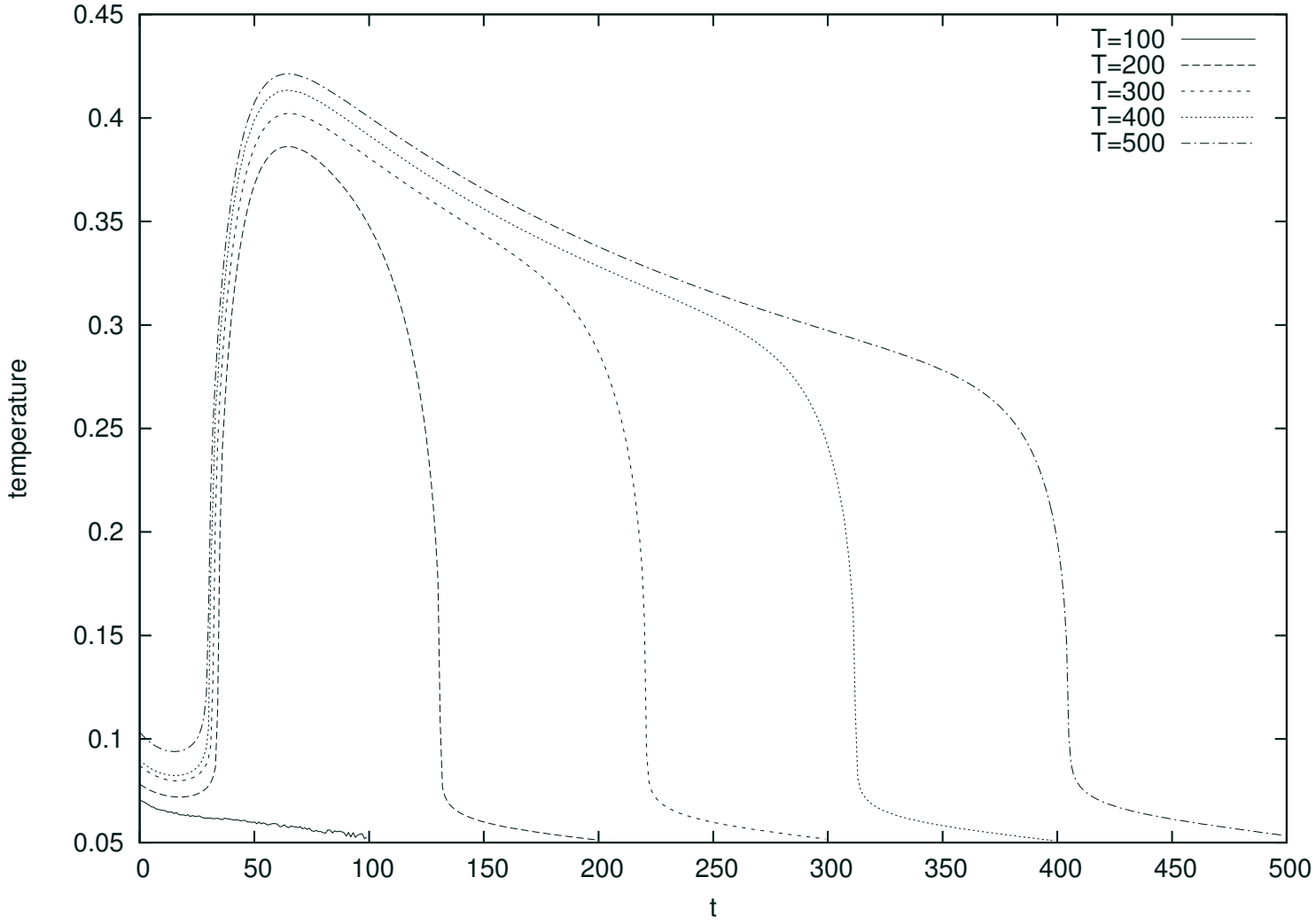
Max-Sat: Annealing Schedules with Where-You-Are



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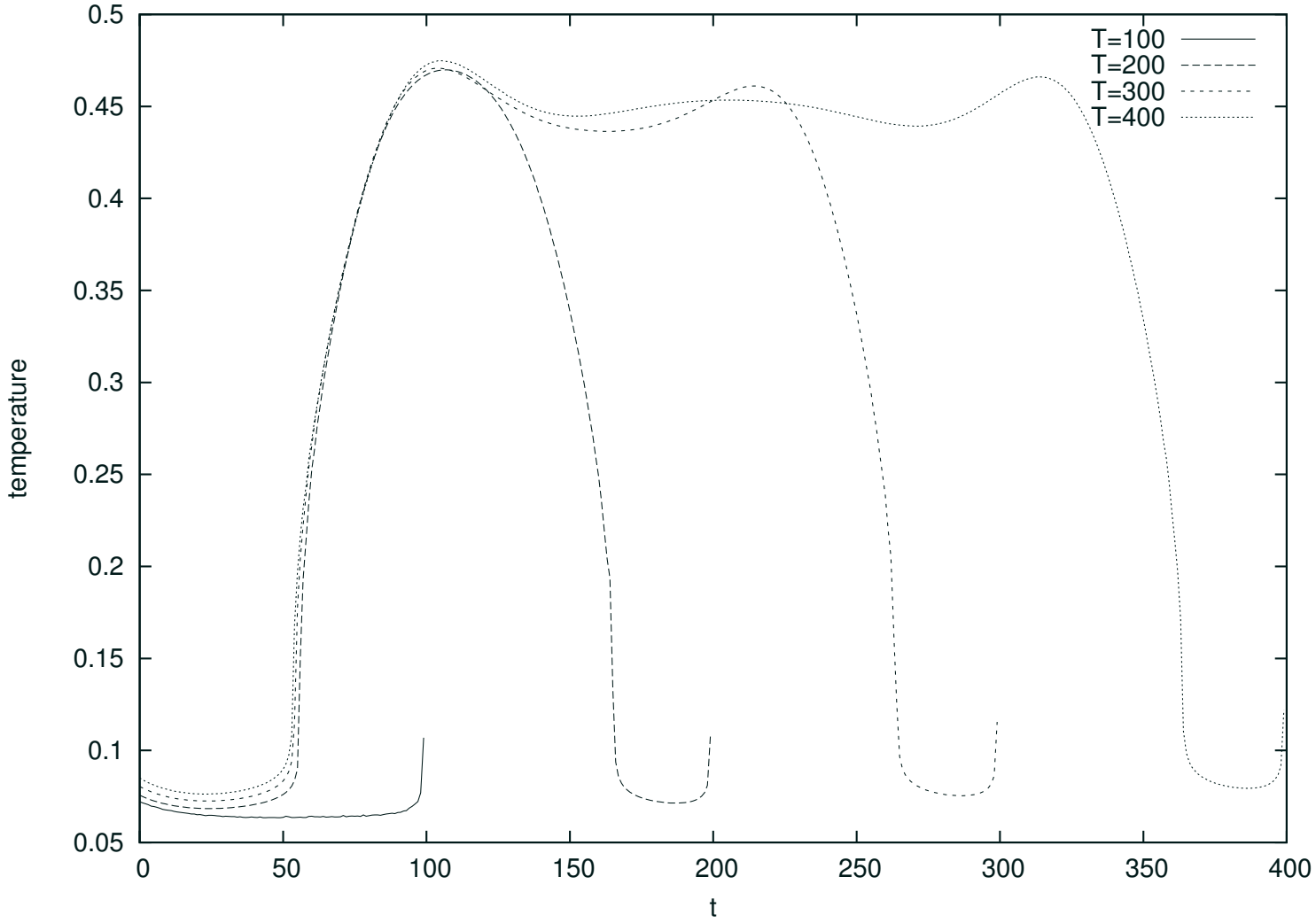
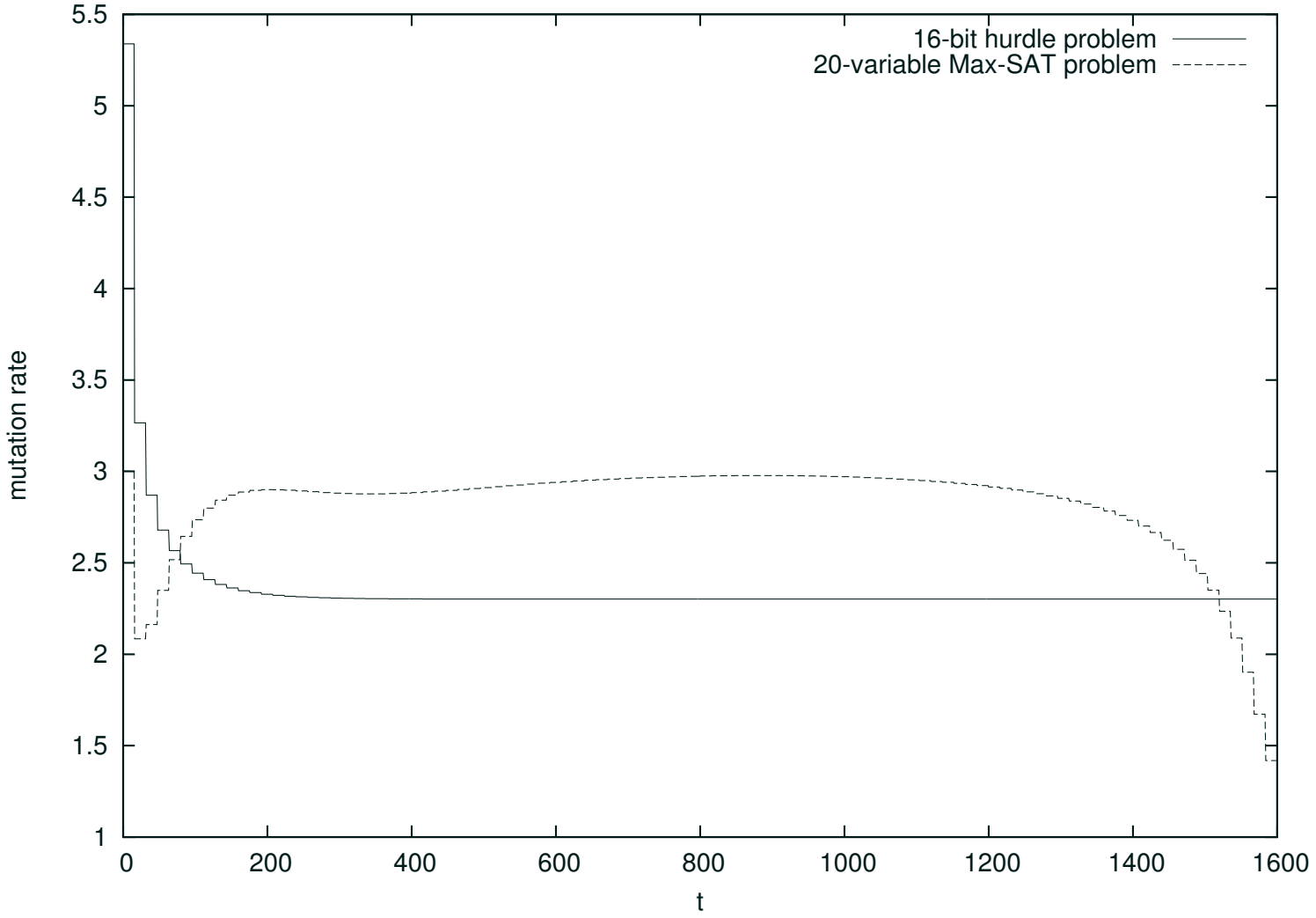


Max-Sat: Mutation Schedule with Where-You-Are



Conclusions

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Any Questions?